Atomic Energy Control Board
P.O. Box 1046
Ottawa, Canada
K1P 5S9

Commission de contrôle de l'énergie atomique
C.P. 1046
Ottawa, Canada
K1P 5S9

INFO-0229

SHALLOW GROUND DISPOSAL - CALCULATION OF DOSE (Assessment of the PRESTO Model to meet AECB Requirements)

by

INTERA Technologies

A research report prepared for the
Atomic Energy Control Board
Ottawa, Canada

Project No. 84.5.15

February 1987

Canada

Research report

SHALLOW GROUND DISPOSAL --
CALCULATION OF DOSE

ABSTRACT

The ability of an existing shallow land burial systems model to meet AECB user requirements has been evaluated. The deficiencies of the program are identified and activities necessary to modify the code to fulfill the user requirements are outlined. Implementation plans for a number of likely scenarios have been constructed and possible cost-cutting measures have been recommended.

RÉSUMÉ

Le présent rapport évalue les capacités d'un modèle de système d'enfouissement peu profond pour satisfaire les besoins des employés de la CCEA qui l'utilisent. Il indique les lacunes du programme et souligne les activités nécessaires pour modifier le code afin de se conformer aux besoins des employés. Le plan de mise en application de certains scénarios possibles a été établi et des mesures possibles pour réduire les coûts ont été recommandées.

DISCLAIMER

The Atomic Energy Control Board is not responsible for the accuracy of the statements made or opinions expressed in this publication and neither the Board nor the author assumes liability with respect to any damage or loss incurred as a result of the use made of the information contained in this publication.

TABLE OF CONTENTS

		Page
ABSTRACT		i
LIST OF TABLES		iv
LIST OF FIGURES		v
1.	INTRODUCTION	1
1.1	Background	1
1.2	AECB User Requirements	2
2.	PRESTO	6
2.1	Overview of Model	6
2.1.1	Development History	6
2.1.2	Processes and Mechanisms	10
2.1.3	Assumptions	31
2.1.4	Limitations	34
2.2	Software Engineering Aspects	35
2.2.1	Documentation	35
2.2.2	Program Structure	38
2.2.3	Extent of Modularity	44
2.2.4	Level of Configuration Control	45
2.2.5	Quality Assurance	46
2.2.6	Verification and Validation History	47
3.	ABILITY TO MEET AECB REQUIREMENTS	50
3.1	Technical Capability	50
3.1.1	Dose Calculations over Time and Space	50
3.1.2	Simulate all Pathways	51
3.1.3	User Selectable Pathways	53
3.1.4	Deterministic and Probabilistic Capability	53
3.1.5	Miscellaneous	54
3.2	Necessary Features	56
3.2.1	User Friendly Input	56
3.2.2	User Controlled Output	57
3.2.3	Modularity	57
3.2.4	Performance on HP1000	57
3.2.5	Self-Teaching Curriculum	58
3.2.6	Restart Capability	58
3.2.7	Execution Error Messages	59
3.2.8	Verified and Validated Program	59
3.3	Summary	60
4.	ACTIVITIES TO MEET AECB REQUIREMENTS	62
4.1	Additional Pathways/Mechanisms	63
4.1.1	Radon Gas Effects	63
4.1.2	Fish and Game Consumption	66

TABLE OF CONTENTS

		Page
4.1.3	Water Exposure Dose	67
4.1.4	Washout for Atmospheric Pathway	68
4.1.5	Surface Water Sediment Effects	69
4.1.6	Snow Shielding Effects	70
4.1.7	Groundwater Contribution to Surface Water	71
4.2	Interactive Input/Output Process	72
4.2.1	Data Input	72
4.2.2	Post-Processing of Results	73
4.3	Probabilistic Capability	73
4.4	Enhanced Modularity	77
4.5	Miscellaneous	78
5.	IMPLEMENTATION PLAN	82
5.1	Possible Scenarios	82
5.1.1	PRESTO and Additional Pathways	83
5.1.2	PRESTO, Additional Pathways and User Friendly Capability	85
5.1.3	PRESTO, Additional Pathways and Probabilistic Capability	85
5.1.4	Full Capability Version	86
5.2	Quality Assurance Procedures	87
5.2.1	Code Modification	87
5.2.2	Verification and Testing	89
5.3	Instruction	89
5.4	Hardware Considerations	90
6.	LEVEL OF EFFORT	91
6.1	PRESTO and Additional Pathways	92
6.2	PRESTO, Additional Pathways and User Friendly Capability	92
6.3	PRESTO, Additional Pathways and Probabilistic Capability	94
6.4	Full Capability Version	94
6.5	Cost Reduction Alternatives	95
7.	CONCLUSIONS AND RECOMMENDATIONS	96
REFERENCES		98
APPENDIX A	Input Variables PRESTO-CPG	
APPENDIX B	ICRP Dose Calculation Methodology	
APPENDIX C	EPA Subroutine Descriptions	
APPENDIX D	Peer Review Panel Comments	
APPENDIX E	Considerations for IBM-PC/AT Version	

LIST OF TABLES

		Page
Table 6-1	Level of Effort for PRESTO Implementation Scenarios (person months)	93

LIST OF FIGURES

		Page
Figure 2-1	PRESTO Model Development	9
Figure 2-2	Pathways and Mechanisms considered in PRESTO	11
Figure 2-3	DARTAB approach for calculating health impacts and doses from environmental exposure (from Begovich et al., 1981)	27
Figure 2-4	PRESTO Program Structure	41

1. INTRODUCTION

1.1 Background

As part of its mandate, the Atomic Energy Control Board (AECB) is required to evaluate an applicant's performance and safety analyses during the licensing process for radioactive waste disposal sites. This report deals with modeling shallow land burial facilities for low-level radioactive waste. The radionuclides contained in such a low-level disposal facility could potentially reach man through a number of pathways. This could include, for example, those radionuclides that would be dissolved and leached by infiltrating water and subsequently removed either by downward percolation or overflow of the facility. Other pathways and mechanisms of interest might include resuspension and deposition of particulate matter in the atmosphere, movement through the surface water system and accumulation in the food chain as appropriate. Because of the complex and coupled nature of these processes, computer models are frequently used to represent the relevant physical and chemical processes that should be considered in an evaluation of a shallow burial facility for radioactive wastes.

As part of its ongoing effort to acquire such technology, AECB has retained INTERA Technologies Ltd. to examine the suitability of one specific computer program, PRESTO, for the evaluation of shallow land burial facilities. More specifically, INTERA was retained to:

1. Determine specific user requirements within AECB;
2. Obtain (with assistance from AECB) the currently available family of PRESTO computer programs;
3. Determine the limiting characteristics of AECB's HP1000 computing system;
4. Assess the software engineering aspects of PRESTO;

5. Evaluate the ability of PRESTO to meet AECB user requirements and its suitability to Canadian conditions;
6. Determine the level of effort and activities required to append software modules to the existing PRESTO computer programs to meet the additional user requirements outlined in 1;
7. Determine the steps to adapt PRESTO to meet AECB user requirements and develop an implementation plan;
8. Document findings in a report.

The selection of PRESTO as the model to be evaluated was based on the results of an earlier study, AECB Research Report INFO-0149, conducted for AECB by INTERA (as GTC Geologic Testing Consultants Ltd.). That study involved undertaking a survey of candidate models (both all encompassing or systems models as well as individual pathway models) for the purpose of selecting the model which most closely met AECB needs. Approximately 200 computer codes were examined before PRESTO was determined as the model most suitable to AECB requirements.

1.2 AECB Requirements and Desired Features

The primary objective in the acquisition of a radioactive waste systems model is to provide the Board with the capability of evaluating the operational and post closure performance of a facility in terms of its ability to meet regulatory requirements. Currently, proposed regulations (AECB, 1986) specify the following dose limits for members of the public:

- the effective dose equivalent received from external sources of radiation plus the committed effective dose equivalent from all prescribed substances entering the body during the year shall not exceed 5 mSv;

- the dose equivalent received by any organ or tissue from external sources of radiation plus the committed dose equivalent to that organ or tissue from all prescribed substances that enter the body during the year shall not exceed 50 mSv.

The following outlines specific user requirements of AECB both in terms of the required technical capability and necessary user features:

1. Calculate the effective dose equivalent to any user specified exposed individual and the collective population dose resulting from the shallow land disposal of Canadian radioactive waste over a user specified period of interest and at a user specified location (receptor);

2. Realistically simulate all potential pathways by which radionuclides may migrate through the environment;

3. Consider only those pathways specified by the user. This capability would allow different sites to be evaluated without having to consider mechanisms/pathways that may not be present at a particular site;

4. Run in either a deterministic or probabilistic mode. This capability would be required to provide a probability distribution function on output parameters enabling a level of confidence to be placed on the results;

5. Include multi-dimensional effects if necessary.

6. User friendly, interactive (preferably menu-driven) entry of input data, including the existence of error checking (e.g., values out of range) and default values;

7. A high degree of modularity to allow the addition, deletion or replacement of modules representing individual pathways/mechanisms;

8. Reasonable processing speed preferably using AECB's HP1000;

9. Fully verified and validated with verification data sets available;

10. Tutorial or self-teaching curriculum;

11. Restart capability to allow a run to continue after a system failure or after a previously defined termination point;

12. User controlled output;

13. Run time error messages in output file.

The above features were identified based on discussions with members of both the Radiation Protection and Waste Management Divisions of AECB. In order to assess PRESTO in the context of the required capability and desired features, the following tasks were undertaken:

1. Review the model processes in the context of their suitability to Canadian shallow land burial facilities. This included any assumptions and approximations that are inherent in the mechanisms used to describe the pathways,

the omission of major mechanisms and/or pathways as well as the existence of any preset (i.e., hard programmed) variables.

2. Review the software engineering aspects of the PRESTO computer code. This involved assessing the program structure, extent of modularity and level of configuration control. In addition, the level of quality assurance to which the computer code has been subjected (including the nature and extent of verification testing) was examined. The quality of documentation describing the model was also reviewed and evaluated.

3. Evaluate the ability of the PRESTO model to meet AECB requirements based on the findings of the previous tasks and an assessment of AECB's in-house computing capability. A recommended course of action was proposed based on the limitations of the program, computing system and the required technical capability and user features.

4. Identify the level of effort associated with those actions required to satisfy all AECB requirements.

2. PRESTO

2.1 Overview of Model

2.1.1 Development History

PRESTO (Prediction of Radiation Effects from Shallow Trench Operations) is a computer simulation model developed primarily for/by the United States Environmental Protection Agency (EPA) to evaluate the possible health effects to humans arising from the disposal of low-level radioactive waste in shallow land burial facilities. PRESTO was originally developed at Oak Ridge National Laboratories (ORNL) with the first version being released in 1981 (Little et al., 1981) and subsequently referred to as PRESTO-EPA. The model was intended to be generic and to calculate the health impacts and exposure to a local static population resulting from the normal releases associated with the post-closure period (up to 1000 years) of a shallow land burial facility. Whenever possible, Little et al. (1981) used existing software in the development of PRESTO-EPA. Typically, these existing software pieces represented all of the physical processes and mechanisms in a particular pathway and were incorporated into the model as a subroutine. Most notable of these existing programs were DARTAB (Begovich et al., 1981), a health effects and dosimetry model, and AIRTRM (a modified version of DWNWND; Fields and Miller, 1980), a Gaussian plume atmospheric transport model.

The second version of PRESTO was released in 1984 (Fields and Emerson, 1984). This version, called PRESTO II by its authors, was also developed at ORNL and was based on the original PRESTO-EPA model but contained more realistic mechanisms to describe infiltration through the trench cap, calculation of trench water balance and groundwater transport through both the vertical region under the trench and the underlying aquifer. This particular version was capable of

analyzing scenarios different from the normal post-closure period, such as intrusion and farming on site. In addition, this version could simulate cap failure due to erosion. This particular version of PRESTO was developed using funding supplied by the United States Nuclear Regulatory Agency (USNRC).

Another version of PRESTO was being developed parallel to, but independently of, the PRESTO II version developed at ORNL. This version, known as PRESTO-EPA-POP was developed from the PRESTO-EPA code of Little et al., 1981. PRESTO-EPA-POP was released in 1985 and incorporated several changes suggested by a Peer Review Panel of PRESTO-EPA. These changes included:

1. The provision of partially saturated conditions from the trench to the aquifer;

2. Modification of leaching option for partially saturated conditions;

3. Modification to the groundwater transport algorithm from local use point to basin stream;

4. Provision of a farming on top of trench scenario;

5. Incorporation of a lag time in the leach process;

6. Revision of the algorithm for calculating radionuclide concentration in vegetation;

7. Decay of radionuclide inventory during operation period;

8. Revisions to output format;

9. Point source changed to an area source for atmospheric transport.

The PRESTO-EPA-POP version formed the basis for subsequent versions of PRESTO such as the PRESTO-EPA DEEP and PRESTO-BRC (Below Regulatory Concern). The PRESTO-DEEP version includes modifications that enable the analyses of three deep geologic disposal alternatives:

1. deep well injection;
2. deep well injection with hydrofracturing;
3. mined cavity disposal.

In addition, the duration of the simulation was extended to 10,000 years. The PRESTO-BRC version was modified to consider the additional exposure pathways that may exist during the operational period of a sanitary landfill that is receiving Below Regulatory Concern (BRC) wastes. The additional exposure pathways include:

1. worker and site visitor dust inhalation during operations;
2. population dust inhalation during operations;
3. population inhalation of incinerator releases;
4. worker and site visitor gamma exposure during operations.

The most recent version of PRESTO is the Critical Population Group (CPG) version. The version was developed by modifying PRESTO-DEEP to calculate a yearly dose commitment based on the use of nuclide and pathway specific dose factors. Other modifications incorporated in PRESTO-CPG include the provision of different classes of wasteforms which have leaching properties.

Figure 2-1 summarizes the development history of the PRESTO model.

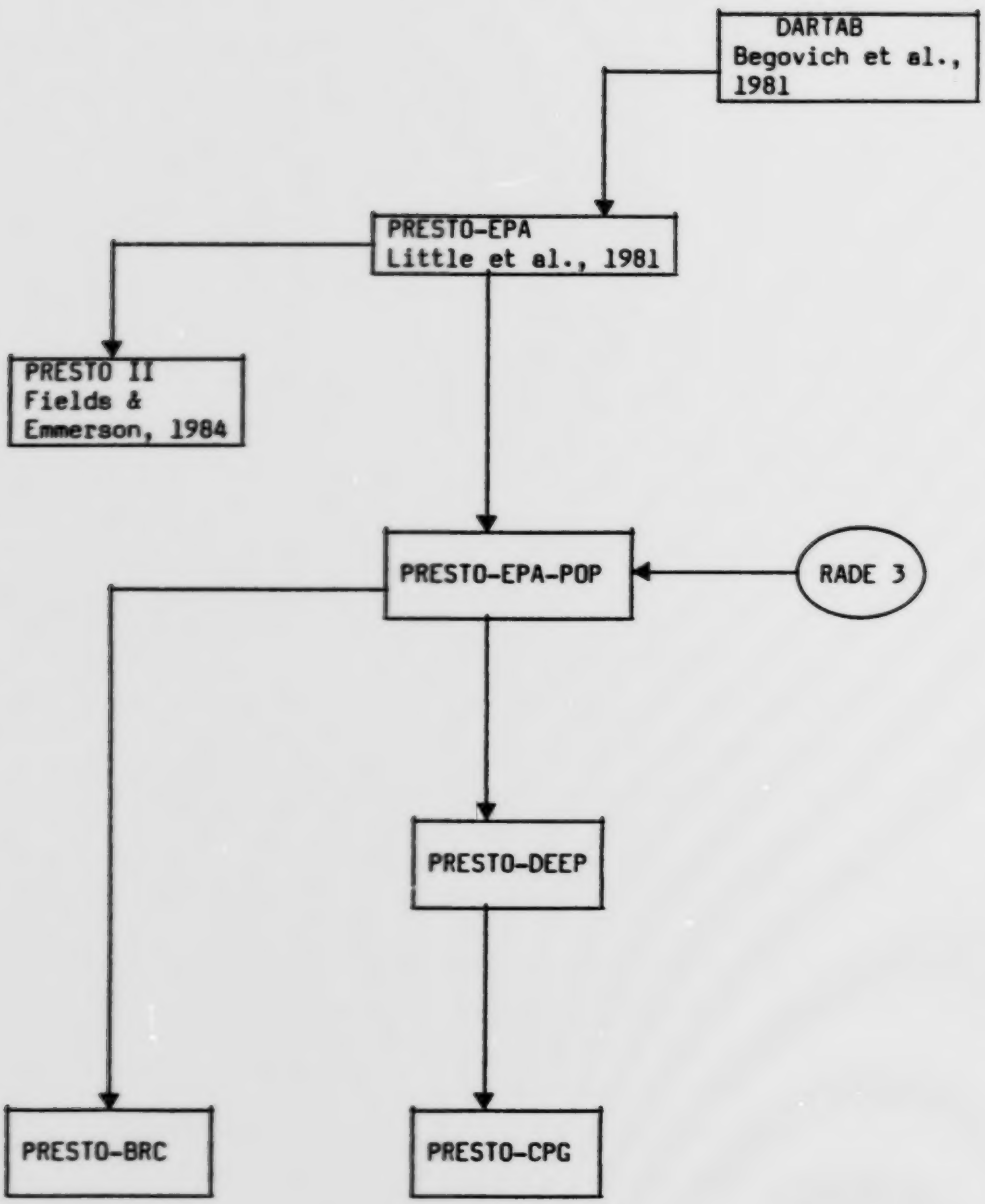


Figure 2-1 PRESTO Model Development
(Prediction Radiation Effects from Shallow Trench Operations)

2.1.2 Processes and Mechanisms

PRESTO was originally intended to simulate the post-closure behavior of a shallow burial facility for low-level radioactive waste. In particular, the model was intended to simulate the impact that the existence of such a facility would have on a local population. This involves the evaluation of the potential for radionuclide migration through a variety of pathways. The major pathways considered within the model may be classified as either hydrologic, atmospheric, or bioaccumulation (i.e., movement through the food chain). All of these pathways have a number of mechanisms associated with them, each of which may control or remove some portion of the radionuclides migrating through a particular pathway. The majority of the pathways considered in PRESTO and the mechanisms associated with them are depicted in Figure 2-2. The scientific approach used by the model in describing these mechanisms is discussed on a pathways specific basis in the following sections. It should be noted that the equations presented are taken from the PRESTO documentation. Although units associated with variables may change between different equations, the necessary conversion is performed in the model. A complete list of input variables for the PRESTO-CPG model is presented in Appendix A.

(i) Hydrologic Pathway

The hydrologic pathway begins with water (some portion of precipitation and irrigation) infiltrating through the overlying cap of the facility. Depending on the rate of infiltration, some or all of the infiltrating water will escape through the bottom of the trench and migrate vertically downwards under either saturated or unsaturated conditions until it encounters an underlying aquifer. The dissolved radionuclides move through the aquifer and at one location may be removed by a well whose water is used for irrigation, watering feedstock, and consumption by the local population. Those radionuclides that are not removed as well water may discharge to a basin (regional) stream where they may be ingested by the regional population. Some of the infiltrating

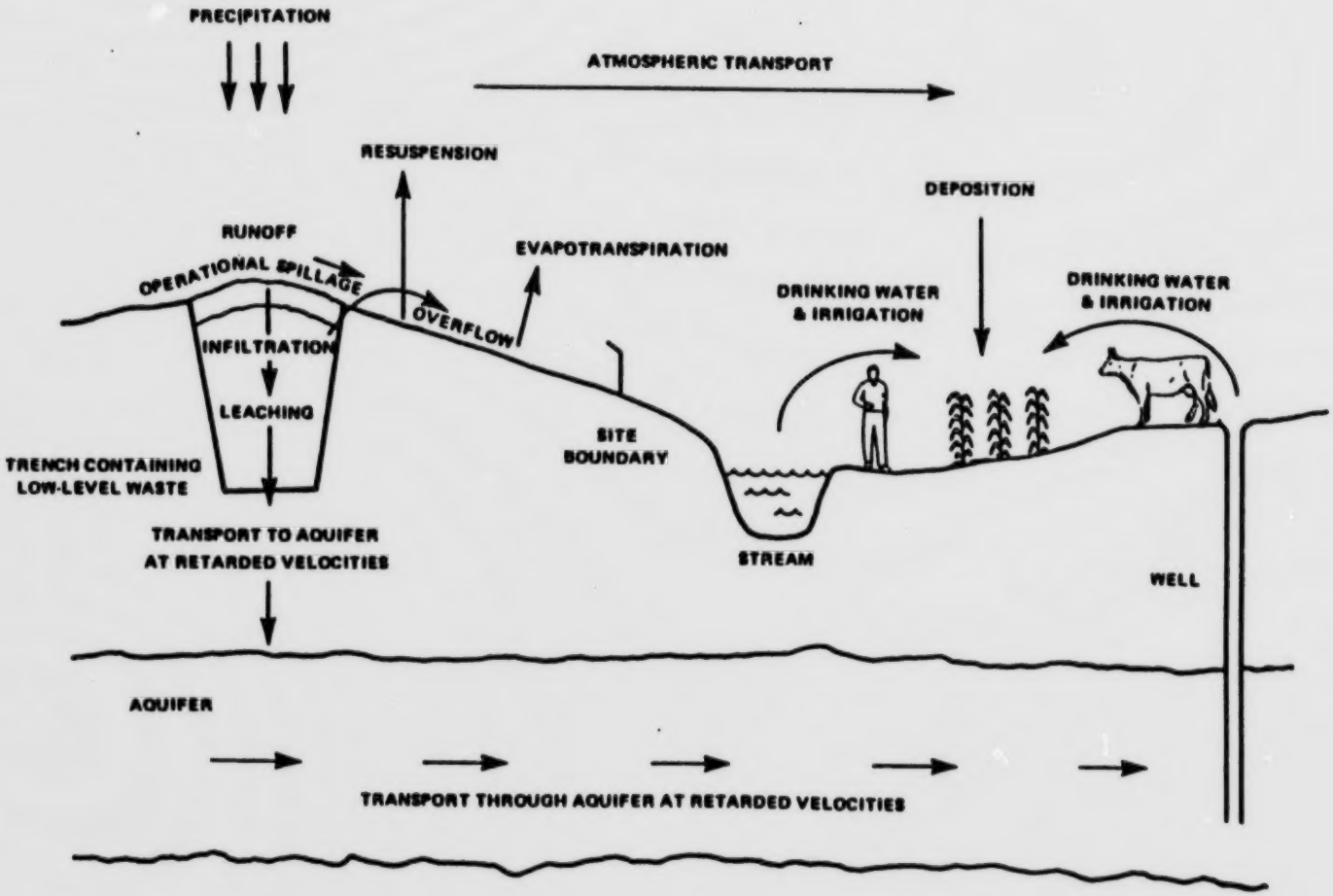


Figure 2-2 Pathways and Mechanisms considered in PRESTO

rainwater may cause the facility to overflow resulting in the removal of dissolved radionuclides. These radionuclides may then either be adsorbed by the active soil layer or removed to a local stream by overland flow. Those radionuclides adsorbed onto the active soil layer are subject to depletion via atmospheric suspension and leaching by rainwater. The leached radionuclides will be transported to the aquifer where they are eligible for removal with well water or by discharging to the basin stream.

The equations representing the movement of radionuclides along these pathways are described in detail in the following sections.

a) Infiltration into Trench from Top

The infiltration into the trench is calculated as the sum of precipitation and irrigation through failed portions of the cap plus percolation through the intact portion of the cap. The percolation through the intact cap is calculated once for an average annual set of conditions using hourly precipitation, daily mean temperatures and monthly maximum day lengths. These meteorologic data are combined with cap properties to calculate the allocation of precipitation among overland flow (runoff), evaporation and percolation.

Infiltration into the top of the cap is calculated by evaluating the various components of the water budget at the cap surface. The amount of water leaving the cap surface as overland flow is calculated using a modified form of Manning's equation:

$$Q_o = \frac{1}{n} \sin^{\frac{1}{2}} \alpha \cdot H^{5/3} \qquad (2.1)$$

where: Q_o = rate of overland flow (m^3/s m);
n = Manning's coefficient ($s/m^{1/3}$);
α = slope of trench cover (degrees);
H = average depth of water (m).

The overland flow equation is used in conjunction with a mass balance to determine the magnitude of other contributions. The mass balance takes the form of:

$$\frac{dH}{dt} = P - E_o - q_o - \frac{Q_o}{L} \qquad (2.2)$$

where: q_o = infiltration into cap (m/s);
P = precipitation (m/s);
E_o = evaporation from overland flow (m/s);
L = ½ trench width (m);
t = time (s).

The evaporation from overland flow is assumed to be equal to the lesser of either the potential evaporation or the sum of precipitation and water in surface storage. Potential evaporation is calculated using Hamons (1981) equation:

$$E_o = CD^2P_t \qquad (2.3)$$

where: C = coefficient (m/sec hr^2);
D = hours of sunshine (hr);
P_t = absolute humidity (unitless).

The above system of equations allows the quantity of water entering into the top of the cap material to be calculated. PRESTO then uses a compartmental type of approach to determine the water distribution within the cap as well as the flux leaving the cap (i.e., entering the trench). The compartmental approach is based on a somewhat idealized discretization of a capillary pressure curve into three types or classifications of water. These include hygroscopic or irreducible water, pellicular water (that held in place by capillary forces) and gravity water (that capable of being removed by gravity forces). Each of these compartments has fluxes and storage capacity associated with

it. The fluxes may be subdivided into water and vapor fluxes. Water fluxes are calculated based on potentiometric gradients and relative permeability while vapor fluxes are calculated based on Fick's (1855) Law. The resulting efflux from the cap is calculated by solving a system of equations based on the water balance of each compartment. This approach is described in detail by Hung (1983).

b) Cap Removal

The trench cap may be removed by either erosion or mechanical disturbance. The mechanical disturbance is entirely user controlled and consists of specifying percentages of areal cap failure at various times.

The erosion process is simulated via a modified form of the universal soil loss equation (USLE, Wischmeier and Smith, 1965):

$$I_L = f_R f_K f_L f_S f_c f_p f_D \qquad (2.4)$$

where: I_L = yearly sediment loss from surface erosion (tons/ha);
f_R = rainfall factor (f_R unit or 100 m·tons·cm/ha);
f_K = soil-erodibility factor (tons/ha/f_R-unit);
f_L = slope-length factor (unitless);
f_S = slope-steepness factor (unitless);
f_c = cover factor (unitless);
f_p = erosion control practice factor (unitless); and
f_D = sediment delivery factor (unitless).

Using this equation, an average annual erosion rate is calculated and is used continuously in the annual time loop until the cap fails (i.e., its thickness is less than 1 cm).

c) Overflow

The water that infiltrates into the trench may either flow out the trench bottom or overflow the trench. While side flow is normally not significant for most disposal operation, this effect may be incorporated (when necessary) by modifying the trench bottom area. The amount of water overflowing the trench is calculated as the difference between that entering the trench and the sum of the storage capacity of the trench and the water exiting the trench bottom (i.e., bottom flux satisfied first). The zone beneath the trench is assumed to be in a constant state of saturation. The user can either specify a saturation level or one will be calculated in accordance with the formula:

$$S = S_r + (1 - S_r) \left(\frac{V_{out}}{K} \right)^{0.25} \qquad (2.5)$$

where: S = saturation (unitless);
S_r = residual saturation (unitless);
V_{out} = average velocity out of trench (m/s);
K = saturated hydraulic conductivity (m/s).

If the user indicates that the material underlying the trench is completely saturated, the flux out of the bottom of the trench is calculated using Darcy's Law:

$$q_{out} = K\, i\, A \qquad (2.6)$$

where: q_{out} = flux out of the trench (m^3/s);
i = gradient (m/m);
A = cross-sectional area (m^2).

For the case at hand, the gradient would be calculated as the sum of the water depth in the trench and the distance to the underlying aquifer divided by the distance to the aquifer.

If the material underlying the trench is partially saturated, the water flux leaving the trench is the same as what enters the trench up to the saturated limit.

d) Leaching

Five different approaches can be used to characterize the release of radionuclides from the waste form. These approaches include specifying either total contact or immersed fraction and either solubility or sorption (i.e., distribution coefficient) controlled. The fifth available option involves a user specified (constant) release rate.

e) Radionuclide Transport through Groundwater

Radionuclide transport calculations are performed for two domains in PRESTO - the vertical reach underlying the trench which is connected to the second domain, the water supply aquifer (assumed horizontal). The approach used to evaluate radionuclide movement through both of these domains is identical, and employs a one-dimensional solution to the convection dispersion equation developed by Hung (1981) and referred to as the "Optimum model". The basic equations for the model as adopted by Hung are:

$$Q = \eta Q_o (T - RD/V) \, \mathrm{Exp}(-\lambda t) \tag{2.7}$$

$$\eta = \frac{\int_0^\infty 0.5(RP/\pi\theta^3)^{\frac{1}{2}} \mathrm{Exp}\{-N_d\theta - (P\theta/4R)(R/\theta - 1)^2\} d\theta}{\mathrm{Exp}(-RN_d)} \tag{2.8}$$

where:

η = a correction factor to compensate for the dispersion effect,
R = retardation factor, R_V or R_H,
P = Peclet number, $V_V D_V/d$ or $V_H D_H/d$,
θ = dimensionless time, $\tau V/D$,
N_d = decay number, $\lambda D/V$,
D = flow length (D_V or D_H),
V = water flow velocity (V_V or V_H),
t = transit time (t_V or t_H),
d = dispersion coefficient (m^2/y),
λ = radiological decay constant (y^{-1}),
τ = dummy time variable,
Q = rate of radionuclide transport at distance D from the source (Ci/yr)
Q_o = rate of radionuclide released at the source, and
T = time of simulation.

The concentration at any point within the aquifer is determined by dividing the rate of radionuclide transport (Q) by the total flow rate across the plume cross section at the point of interest.

f) Surface Contamination

Contamination of the upper soil surface may originate from two mechanisms: surface spillage and/or trench overflow. The surface spillage arises from disposal operations and hence is specified (by user) in place initially. These radionuclides as well as those added subsequently by trench overflow are assumed to be contained in a finite (user specified) active soil layer. The soil layer contains both soil and water and the radionuclides within this zone are partitioned between these media through the use of a distribution coefficient, i.e.,

$$C_W^S = \frac{10^3 I_S}{K_{d_1} M_S + M_{W_2}/\rho_W} \qquad (2.9)$$

where:

C_w^s = radionuclide concentration in surface soil water (Ci/m³),
I_S = amount of radionuclide on surface (Ci),
K_{d_1} = distribution coefficient for surface soil region (ml/g),
M_S = mass of soil in contaminated region (kg),
M_{w_2} = mass of water in contaminated soil region (kg),
ρ_W = density of water = 1 g/cm³, and
10^3 = conversion factors used for K_d(1 ml/g = 1 m³/10³ kg) and for ρW (1 g/cm³ = 10³ kg/m³).

Water entering into the active soil zone may leave as either overland flow or as percolation/recharge to the groundwater system. The amount of overland flow is user specified as a fraction of precipitation while the amount of groundwater recharge is specified by a farmland infiltration parameter. Although the sum of overland flow and infiltration should realistically not exceed total precipitation, the model (as discussed in Section 3.2.1) will not invoke this constraint.

g) Stream Contamination

The local stream is assumed to have only one source of radionuclide contamination - overland flow. The mass of radionuclides being transported to the stream (R_S) is the product of overland flow (W_S) and water concentration in the active soil zone (C^S_W):

$$R_S = C^S_W \times W_S \qquad (2.10)$$

The concentration of radionuclides in the stream is equal to the mass of radionuclides divided by a user specified steam flow.

(ii) Atmospheric Processes

The atmospheric pathway commences with the suspension of radionuclide particulate matter from the active soil zone. This material is subsequently transported through the atmosphere using a Gaussian plume model and may be removed by dry deposition. Washout due to rain, however, is not considered. A variety of formulations are available to describe the dependence of dispersion parameters on the distance from the source to the receptor. The following sections describe the equations employed to simulate atmospheric processes.

a) Source Term

Only one source of radionuclides is considered for atmospheric transport, the portion of radionuclides adsorbed onto soil particles. The source term is calculated based on a time dependent suspension factor and/or a mechanical (process dependent) suspension factor. The time dependent factor is meant to represent a wind driven component and is represented by:

$$Q_r = C_A H_D U F \sqrt{A} \qquad (2.11)$$

where: Q_r = suspension rate (gm/s),
C_A = atmospheric concentration (gm/m^3),
H_D = mixing length (m),
U = wind speed (m/s),
F = correction factor,
A = area of source (m^2).

A number of these parameters are calculated using other relations:

$$F = \frac{V_g \sqrt{S_L S_w}}{U H_D} \qquad (2.12)$$

where: V_g = gravitational fall velocity (m/s);
S_L = length of source (m);
S_w = width of source (m).

and

$$C_A = Re\ C_s^s \rho_s S_D 10^3 \qquad (2.13)$$

where: Re = empirical factor (after Anspaugh et al., 1975) (1/m);
ρ_s = density of soil (kg/m^3);
C_s = concentration of sorbed radionuclide (gm/gm);
S_D = depth soil zone (m).

The second mechanism contributing to the source term is mechanical disturbance characterized by:

$$Q_{mech} = ARF_{mech} C_g \qquad (2.14)$$

where: $C_g = C_s\ \rho_s\ S_D\ 10^3$;
R = resuspension factor (1/s);
F_{mech} = fraction of year mechanical disturbance present (unitless);

b) Atmospheric Transport

The PRESTO program performs atmospheric transport using a Gaussian plume model of the form:

$$x = \frac{Q}{2\pi u \sigma_y \sigma_z}\left\{\exp\left[-\frac{y^2}{2\sigma_y^2}\right]\right\}\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \qquad (2.15)$$

where: χ = radionuclide concentration (gm/m^3);
Q = source strength (gm/sec);
U = wind speed (m/s);
σ_y, σ_x, σ_z = dispersion parameters (m);
y,z = co-ordinates (m);
H = source release height (m).

The model as programmed in PRESTO assumes reflection of the plume at the ground surface and assumes that the population resides in one user specified 22.5° sector. Air concentrations are calculated using average annual meteorological conditions. Dispersion parameters may be calculated by several formulations including Briggs (1973) and Moore et al. (1979) although the formulation of Pasquill (1961) is recommended. A correction factor, based on user supplied depositional information, is also incorporated into the atmospheric transport equation to account for losses due to dry deposition.

iii) Food Chain and Dose Calculations

Dose to an individual may arise from a variety of mechanisms. Those mechanisms considered by PRESTO include:

1. Ingestion of contaminated food stuffs and water;
2. Inhalation of contaminated air/particulates;
3. External exposure to contaminated air and soil surfaces.

The dose due to ingestion will be a function of the bioaccumulation in vegetation and livestock as well as radionuclide concentrations in the drinking water. As with the dose contribution from inhalation and external exposure, a dose conversion factor is used to relate radionuclide concentrations to doses. The following sections describe the methodology used by PRESTO to calculate radionuclide concentrations in food stuffs and doses to man.

a) Food Chain

The following equation is used by PRESTO to calculate the concentration (C_v) of all radionulides (except ^{14}C and ^{3}H) in and on vegetation:

$$\bar{C}_v = \left\{ \frac{d\ R[1-\exp(-\lambda_e t_e)]}{Y_v \lambda_e} \right\} + \frac{B \cdot CSP}{P} \exp(-\lambda t_h) \qquad (2.16)$$

where: $\bar{C}_v$ is measured in pCi/kg, d is defined below, and

R = the fraction of deposited activity retained on crops (unitless).
λ_e = effective removal rate constant for the radionuclide from crops (h^{-1}), where $\lambda_e = \lambda + \lambda_w$, λ is the radioactive decay constant, and λ_w is the removal rate constant for physical loss by weathering.
t_e = the time period that crops are exposed to contamination during the growing season (h).
Y_v = the agricultural productivity (yield) [kg(wet weight)/m^2].
B = the radionuclide concentration factor for uptake from soil by edible parts of crops. [pCi/kg (wet weight) per pCi/kg dry soil].
CSP = soil radionuclide concentration, updated yearly (pCi/m^2).
P = the effective "surface density" for soil [kg(dry soil)/m^2], and
t_h = time interval between harvest and consumption of the food (h).

and

$$CSP = (CSPL+d)\exp(-\lambda-\lambda_s) \qquad (2.17)$$

where CSP = soil radionuclide concentration for this year (pCi/m^2).
CSPL = soil radionuclide concentration for last year (pCi/m^2).
d = mean rate of radionuclide deposition (pCi/m^2-yr).
λ = radioactive decay constant (yr^{-1}), and
λ_s = rate constant for contaminant removal (yr^{-1}).

The atmospheric deposition rate onto food surfaces or soil is calculated in PRESTO as:

$$d = \bar{C}_A V_d \cdot 3.6X10^{13} \qquad (2.18)$$

where:

d = mean rate of radionuclide deposition onto ground or plant surfaces (pCi/m²·h),
$\bar{C}_A$ = mean ground level radionuclide concentration at point of interest (Ci/m³),
$3.6X10^{13}$ = sec·pCi/h·Ci, and
V_d = deposition velocity (m/sec).

Equation (2.16) can be used to calculate the concentration in vegetation due to irrigation with contaminated water. For irrigation, the deposition rate becomes the irrigation rate.

The rate constant for contaminant removal from the soil, λ_S, is estimated using:

$$\lambda_S = \frac{r_S}{(0.15)(8760)\left(\frac{1+\rho_S k_d}{\theta_S}\right)} \qquad (2.19)$$

where:

λ_S = removal rate coefficient (h^{-1}),
r_S = watershed infiltration (m/y),
ρ_S = soil bulk density (g/cm³),
k_d = distribution coefficient (ml/g),
θ_S = porosity (unitless),
0.15 = depth of soil layer (m), and
8760 = h/y.

Equation (2.16) is used to calculate vegetation concentrations for all plants including pasture grass and livestock feed. These latter two quantities are used together with dietary fractions to calculate a concentration in the animal's feed (C_p). The radionuclide concentration in meat is estimated by:

$$C_F = F_f(C_f Q_f + C_w \cdot Q_w)\exp(-\lambda t_s) \qquad (2.20)$$

where:

C_F = the nuclide concentration in animal flesh (pCi/kg).
F_f = the fraction of the animal's daily intake of a given radionuclide which appears in each kilogram of flesh (d/kg).
C_f = the concentration of radionuclide in the animal's feed (pCi/kg).
Q_f = the amount of feed consumed by the animal per day (kg/d), and
t_s = the average time from slaughter to consumption (h).
C_w = concentration in water (pCi/L),
Q_w = rate of water consumption (L/day).

It should be noted that the constant F_f (and F_m below) are used to represent the net accumulation in the foodstuff. The radionuclide concentration in milk is calculated using a similar methodology:

$$C_m = F_m(C_f Q_f + C_w \cdot Q_w)\exp(-\lambda t_f) \qquad (2.21)$$

where:

C_m = concentration of tritium in milk (pCi/L).
F_m = fraction of the animal's daily intake of ^3H that appears in each liter of milk (days/l).
C_w = ^3H concentration in animal's drinking water (pCi/L).
Q_f = animal's daily intake of forage (kg/d).
Q_w = cow's daily intake of water (l/d).
C_F = concentration of tritium in animal's flesh (pCi/kg). and
F_f = fraction of the animal's daily intake of ^3H that appears in each kg of flesh (d/kg).

The calculation of ^{3}H and ^{14}C concentrations in foodstuffs requires additional assumptions/equations. In the case of ^{3}H it is assumed that the irrigation contribution to the total concentration of the vegetation is equal to that of the irrigation water. The equation is also further simplified by neglecting the decrease due to radioactive decay.

For vegetation contaminated by atmospheric deposition of tritium, the ^{3}H contribution to the total concentration is calculated by:

$$C_v = \frac{C_A}{h}(0.75)(0.5)(1x10^{15}) \qquad (2.22)$$

where: C_v = tritium concentration in vegetation (pCi/kg).
C_A = concentration of ^{3}H in air (Ci/m^3).
h = absolute humidity of the atmosphere (g/m^3).
0.75 = fraction of the plant mass that is water.
0.5 = ratio of tritium concentration in plant water to that in atmospheric water, and
$1x10^{15}$ = ($1x10^{12}$pCi/Ci)x(10^{3}g/kg).

The ^{14}C concentration of vegetation is assumed to be attributable solely to atmospheric concentrations and can be calculated from:

$$C_v = \frac{C_A r}{0.16}(0.11)(1x10^{15}) \qquad (2.23)$$

where: C_v = carbon-14 concentration in vegetation (pCi/kg).
C_A = mean ground-level concentration of ^{14}C in air (Ci/m^3), also calculated from equations given in Sec. 2.2.2.
r = ratio of the total release time of ^{14}C to the total annual time during which photosynthesis occurs.
0.11 = fraction of the plant mass that is natural carbon, and
0.16 = concentration of natural carbon in the atmosphere (g/m^3).
$1x10^{15}$ = ($1x10^{3}$pCi/Ci)x(10^{3}g/kg)

b) Dose Calculations

PRESTO calculates the dose contribution via four pathways: ingestion, inhalation, air immersion and ground surface exposure. The following description of the PRESTO methodology used for dose calculations is based on the description provided in Begovich et al., 1981. The described DARTAB program combines environmental exposure data and dosimetric and health effects data to calculate doses and evaluate heath impacts. An example is illustrated in Figure 2-3 in which the environmental exposure data is calculated by AIRDOS-EPA and the dosimetric and health effects data to be used by DARTAB is calculated by RADRISK. The current version of PRESTO performs the environmental exposure portion of the code. The dosimetric and health effects data are read from input files and, as such, need not be those generated by RADRISK but could be user supplied for instance AECB staff may want to use ICRP's latest data.

A) Dose to an Organ

The dose (D) arising to any organ (l) from any nuclide (i) over a specific pathway (j) is calculated as:

$$D_{ijl} = \frac{C_j E_{ij(k)} \cdot DF_{ijl}}{P(k)} \qquad (2.24)$$

where: D_{ijl} = annual organ absorbed dose (mrad/yr),
C_j = units conversion factor for pathway,
$E_{ij}(k)$ = annual population exposure for pathway j, from nuclide i, at location k,
DF_{ijl} = dose conversion factor,
$P(k)$ = population exposed at location k.

The units of exposure and dose conversion factor are dependent upon the pathway. Exposures $E_{ij}(k)$ are calculated from user specified intake rates. Exposures due to ingestion are calculated as the sum of the intake for each radionuclide from contaminated vegetation, milk,

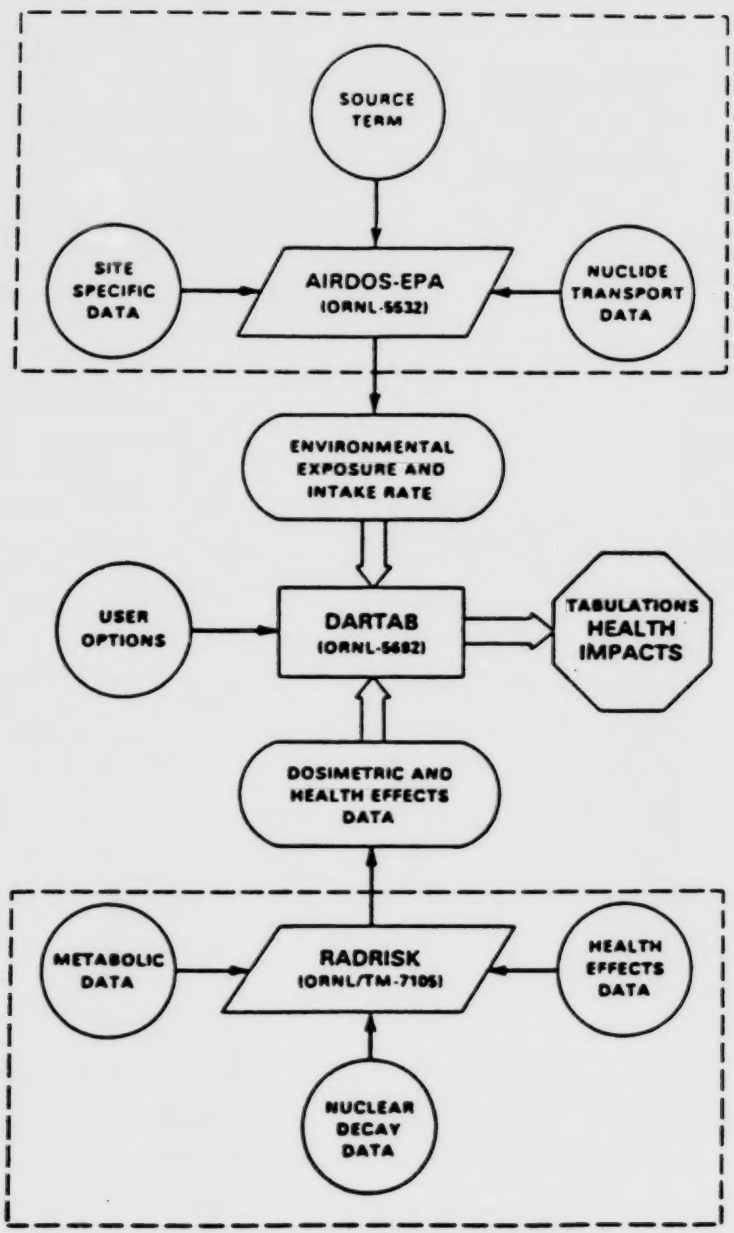


Figure 2-3 DARTAB approach for calculating health impacts and doses from environmental exposure (from Begovich et al., 1981)

meat and water. Inhalation exposures are calculated by taking the product of a breathing rate and mean ground level air concentration for each radionuclide. Air immersion doses are calculated from air concentrations while external doses are calculated from contaminated soil due to irrigation and atmospheric deposition.

The dose equivalent (mrem), H, for the 1th organ is given as:

$$H_1(k) = QF(\text{low-LET})XD_1(k.\text{low-LET}) + QF(\text{high-LET})XD_1(k.\text{high-LET})^* \quad (2.25)$$

where QF denotes the quality factor.

B) Dose to the Whole Body (effective dose equivalent)

To combine dose rates to different organs (e.g., obtain an effective dose), a weighted sum is used:

$$D_{ij} = \sum_1 W_1 D_{ij1}(k) \quad (2.26)$$

where: W_1 are weighting factors for the various organ doses and,

$$\sum_1 W_1 = 1 \quad (2.27)$$

Weighting factors and dose conversion factors developed by EPA for the various organs are used as input into PRESTO. However, it is possible to replace these EPA values with other user specified values.

C) Dose to a Population

It should also be noted that although EPA claims that PRESTO calculates a population dose, this population is assumed to reside at one location. A collective dose as defined by ICRP is not calculated. Differences between the EPA approach to dose calculation and AECB procedures are documented in Appendix B.

PRESTO also performs extensive health risk and risk equivalent calculations using a methodology that is analogous to the calculation of dose (i.e., use of risk factors for various organs).

*Note: LET = Linear Energy Transfer Radiation

(iv) Additional Features

In addition to the normal post-closure calculations of dose to a local population PRESTO may be used to perform alternate calculations. These alternate calculations include mainly the dose to an individual arising from a number of special scenarios. These scenarios include the dose to a resident intruder and the dose from farming over the trench. The following sections describe each of these scenarios in detail.

The major differences between the resident intruder scenarios and the normal operational scenario are contained in the methodology/assumptions used in calculating the external exposure dose. An additional contribution to this dose is added to that obtained from the contaminated ground surface to reflect the additional exposure resulting from the construction of a basement into the disposal trench. This calculation is performed by comparing the dose obtained in a basement to that obtained while standing on contaminated ground and using a conversion factor (having units of length) to relate the two quantities. This approach is based on a number of assumptions:

- the basement is circular of 3 m radius;
- on average an individual spends 1/3 of his time in the centre of the basement;
- attenuation coefficients of the trench equal those of soil.

The conversion factor is a function of the gamma energy associated with the decay process. Following an investigation of a range of energies a conservative value of 0.1 m was hard programmed in the PRESTO basement exposure calculations.

Farming may take place on-site or off-site, with on-site farming being either directly in the waste or in the overburden covering the waste. The only difference between the algorithms used to calculate foodstuff concentrations for the different scenarios is in the methodology of determining soil concentrations. Off-site the concentration of radionuclides within the soil is calculated based on the deposition of radionuclides from irrigation water and the atmosphere. The soil concentration of the active soil zone (i.e., that from overflow and spillage) is used when farming is conducted in the overburden of the trench. If farming within the trench material is specified then the concentration of radionuclides within the soil is assumed equal to the mass of radionuclides in the trench divided by the depth of an active surface zone.

The output from PRESTO may also be used by a post-processor (known as the Accounting Model) to perform dose calculations to a basin or regional population. Unfortunately, at the time of this writing no detailed documentation describing this post-processor was available. It is known that the assumptions inherent in the dose calculation for the regional model include ignoring the contribution from all pathways except the hydrologic and assuming the contamination in the basin river is due solely to groundwater discharge.

It should be noted that these scenarios (i.e., farming on trench, intruder, normal operation) are mutually exclusive, that is only one scenario may be simulated per execution run.

PRESTO-CPG may also be used to evaluate disposal configurations other than shallow land burial, including deep well injection, hydrofracturing and deep geologic disposal. A number of shallow burial mechanisms will be ignored if any of these configurations are selected. Those mechanisms that are ignored include the infiltration process for all three deep scenarios and the atmospheric transport mechanism for deep geologic disposal. One additional transport mechanism is introduced to account for the vertical upward migration of

radionuclides from the disposal site to an overlying horizontal aquifer. The other major feature of these deep scenarios that is distinctive is the treatment of leaching of the radionuclide inventory. Both the hydrofracturing and deep disposal use a release rate fraction while the deep well injection option uses an equilibrium based methodology.

2.1.3 Assumptions

The majority of the assumptions present in PRESTO may be classified in either of two categories. The first category contains those assumptions regarding the disposal site and pathway configurations as well as which equations can be used to adequately represent the process/mechanisms present in these pathways. The second category of assumptions pertains to the use of specific values in the selected equations. Examples of assumptions belonging to the first category include:

- the use of Mannings Equation to calculate overland flow;
- soil erosion can be calculated by the Universal Soil Loss Equation;
- the population is static;
- groundwater contributions to the local stream are negligible;
- annual average meteorological values can be used to represent long term conditions;
- the contribution of daughter products is either not significant or can be included through secular equilibrium;
- contributions to dose are primarily from ingestion (of vegetation, milk, water and meat), inhalation, exposure to contaminated ground and air;

- equilibrium distribution coefficients adequately represent the geochemical interaction between radionuclides, water and soil;
- a particulate Gaussian plume model that considers only dry deposition is adequate to model airborne transport of radionuclides;
- dose is a linear function of exposure (i.e., dose factor methodology holds);
- the only engineered feature of the disposal facility is a cap that is subject to removal by erosion.
- ^{14}C contribution in vegetation is assumed to be due solely to atmospheric sources;
- ^{3}H concentration in vegetation is assumed equal to that of drinking water;
- regional or basin doses are due solely to residual nuclides of the hydrologic pathway;
- vertical and horizontal air dispersion parameters are described by the relationship of Pasquill (1976).

In addition to this first category of assumptions there exist a number of fixed parameters. The code changes necessary to make these values user specified are dicussed in Chapter 4. The fixed values include:

- the population is assumed to reside in a 22.5° sector for the purpose of air quality calculations;
- Mannings "n" is set to 0.05;
- the moisture profile under the trench is fixed in accordance with the equation described in Section 2.1.2;
- the time step of the main time loop is fixed at one year;
- for the resident intruder the basement is assumed to be of 3 m radius and occupied 1/3 of the time;
- the streamflow for the regional (basin) stream is sized based on the assumption of an annual river flow to population ratio of 3000 m^3/capita;
- cap failure occurs when the thickness is less than 1 cm;

- the depth of the active soil zone is 15 cm;
- an irrigation rate of 4492 m^2/person is assumed;
- the volume of water consumed by cattle on a per person basis is 15000 L/person yr;
- 37.8% of cattle feed is composed of reproductive portions of plants with the remainder coming from vegetative portions;
- a translocation factor of 0.1 is assumed for produce (excluding leafy vegetables) consumed by man for all radionuclides except ^{3}H and ^{14}C;
- a release height of 1 m is assumed for atmospheric releases;
- plant mass is assumed to be 75% water;
- the amount of tritium in atmospherically derived plant water is assumed to be 50% of the atmospheric concentration;
- plant mass is assumed to be 11% natural carbon;
- the natural carbon concentration of the atmosphere is 0.16 gm/m^3;
- a 90 day time lag is assumed for the consumption of stored feeds;
- snowmelt coefficient of 3.05 mm/°C day is assumed;
- hard programming of a number of fresh to dry weight conversion factors for food and animal feed.

In addition to the values assumed above PRESTO contains other types of hard programmed variables. These include conversion factors for units, pre-set iteration limits and tolerances and default values. Default values include:

- average age of 70.7 yr;
- height of inversion lid equal to 1200 m;
- population replacement rate of 0.0141/yr;
- ground surface correction factor of 0.5.

2.1.4 Limitations

The limitations of PRESTO are, for the most part, associated with the assumptions described in the previous section. For example, PRESTO is subject to the following limitations:

- Relatively long simulation periods: Due to the inclusion of equilibrium sorption methodology and linear dose conversion factors, short term (i.e., significantly less than one year) and acute simulations are not feasible. Fixed time step also means that time periods less than one year cannot be examined.

- Meteorological parameters constant: Effects of variation in meteorological parameters over a time sequence cannot be examined.

- No contribution of gaseous radionuclides (e.g., radon): Only particulate radionuclides considered with PRESTO.

- Relatively flat terrain: Gaussian plume model and dispersion parameters are not suitable for locations such as mountains and canyons.

- Fish and game are not significant fractions of total diet: PRESTO does not include the dose arising from these sources.

- Contribution to dose by long-lived (relative to parent) daughter products must be insignificant: PRESTO does not consider decay chains.

- One receptor location: PRESTO considers only one (constant) user specified location for each of well location, stream location and residence.

- Population distribution/density does not change significantly over simulation time.

- No accumulation or decay of radionuclides in surface water bodies: Stagnant water bodies cannot be considered.

In addition, a number of limitations exist that are associated with the scope of PRESTO. For example, the model does not consider such low probability high consequence events such as flooding, earthquakes, etc. As such, PRESTO is limited to normal operations or the resident intruder and farming scenarios.

2.2 Software Engineering Aspects

2.2.1 Documentation

The current documentation describing PRESTO is contained primarily in two reports, one entitled "PRESTO-EPA-POP: A Low-Level Radioactive Waste Environmental Transport and Risk Assessment Code - Methodology Manual" and the other "PRESTO-EPA-POP: A Low-Level Radioactive Waste Environmental Transport and Risk Assessment Code - Users Manual". The first of these documents describes the scientific basis of PRESTO, the equations used in simulating the pathways/mechanisms of interest, and the underlying philosophy of the model as well as a general description of the code and its output. The second report is strictly a users manual and describes input variables and their required format, types of output tables, examples of both as well as a sample job control language (JCL) stream. As mentioned previously, these reports form the

primary source of information for PRESTO. Additional reports describing PRESTO versions DEEP, BRC and CPG are available but are relatively short and merely describe the modifications made to the POP version.

It should be noted that the documentation that was reviewed as part of this study was in draft form and that the final document may be significantly different and the criticisms voiced herein may be subsequently amended. The two primary reports describing PRESTO are quite large totalling over 250 pages. However in spite of their size, it would appear that some significant deficiencies exist in their description of the PRESTO program. These deficiencies include:

- Inadequate description of the assumptions/approximations present within the code and their associated limitations. For example, the decay of radionuclides in either of the surface water systems is not considered. This aspect of the model is neither identified nor are the possible ramifications (if any) of such an omission discussed.

- Omissions in the form of mechanisms/processes present within the code. For example, the infiltration routine performs a check on temperature to identify whether the precipitation is rain or snow. If the temperature remains below 32°F the snow is allowed to accumulate and the calculation of infiltration is by-passed. If the temperature is greater than 32°F, the volume of snowmelt is calculated using an incremental temperature and a snowmelt coefficient.

- Errors in input data. The spelling of several namelist variables was inconsistent between the documentation and the code itself. In addition at least one input variable was omitted from the data list described in the users manual.

- Incomplete discussion of hard programmed variables. PRESTO contains a number of hard programmed variables all of which make some assumption regarding a process. Some of these variables (such as the quantity of irrigated land per person of 4492 m^2/person) are identified within the documentation although references substantiating the value typically are not given. In other instances, such as the case of Mannings "n", a value of 0.05 was merely hard programmed into the code, an item which was not mentioned in the documentation.

- Poor or non-existent description of the coupling that may (or should) exist between various processes. For example, water falling as rain will either infiltrate, evaporate or runoff. Both the infiltration rate and overland flow (runoff) are functions of the depth of ponding which is itself dependent on the removal rate of the three processes. There are therefore, a number of possible ways of solving the equations describing these processes e.g., explicit, implicit, semi-implicit, each of which has certain limitations/advantages associated with it. This level of information is not presented in PRESTO.

- Confusing nomenclature. For example, two different surface water bodies are referred to as streams (i.e., both a local and basin stream) although the adjectives local and basin are frequently dropped. In addition, the basin stream is sometimes referred to as a river.

- Organization poor. Often important information is misplaced. For example, the fact that the dose contribution due to consumption of fish is assumed to be negligible for the local population is presented only in

the section on regional health effects. Similarly the fact that the model uses a fixed one year time step is stated only in the executive summary.

- Documentation not concise. Although a significant quantity of technical information is presented in the PRESTO documentation, it is difficult to extract the information from the text. In many instances, the pertinent information is deeply embedded in the text and it is only by reading the entire report very carefully that the information can be discerned. The report could have been written in a clearer and more concise manner.

Although the above criticisms may sound severe, it must be pointed out that the reviewed report is still in draft format. However, it is believed the final report could be much improved through incorporation of these suggestions.

2.2.2 Program Structure

In developing PRESTO, EPA tried to fulfill several basic design objectives. These objectives include:

1. the use of existing release and pathway submodels where possible to reduce development time and costs;

2. use of a modular design to allow the insertion of an alternate submodel where required;

3. ability to run economically;

4. flexibility to allow the analysis of a wide range of climatic, waste and engineering configurations;

5. use of EPA's health risk methodology;

6. a program capable of providing realistic, reliable and verifiable results.

The resulting software configuration reflects, to some extent, the constraints imposed by the design objectives. PRESTO makes extensive use of existing software. For example, the dose to man and health risk calculations are performed using a program known as DARTAB (Begovich et al., 1981) which was incorporated into PRESTO as a subroutine. DARTAB also uses the results of another program, RADRISK (Dunning et al., 1980) as an input file. The air transport portion of PRESTO was also originally a separate program known as DWNWND (Fields and Miller, 1980) and was also incorporated as a subroutine. The effect of using these programs as part of PRESTO is clearly evident in the resulting code. Programming styles vary widely in various portions of the code with some portions of the code being well programmed (i.e., efficiently, intelligently) while other portions exhibit poor programming practises.

In particular, the DARTAB portion of PRESTO contains some significant examples of poor programming practises. They include:

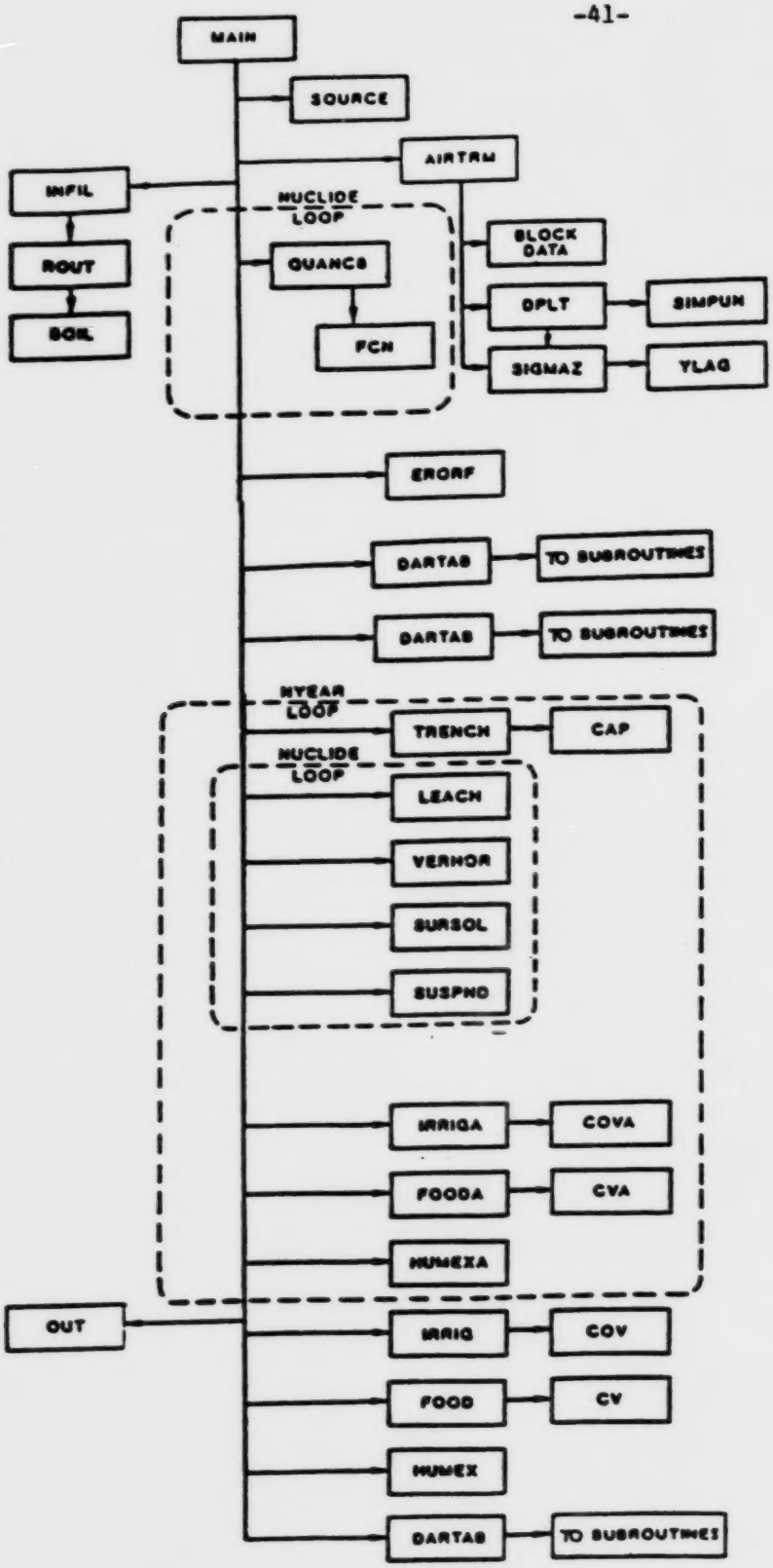
- use of namelist input (poor from the standpoint of machine compatability);
- logic which transfers program control to the middle of a "Do-Loop";
- subroutine to subroutine inconsistencies in labelled common blocks (both variable typing and total size);
- use of character values in integer, real, and double precision real variables.

The remainder of PRESTO also has its own examples of poor programming practises:

- use of hard programmed variables for I/O units;
- inconsistent placement of format statements;
- use of hard programmed constants when a variable already exists;
- nearly duplicate subroutines.

A trade-off exists when previously developed software is used in the development of a new program. As indicated in EPA's design objectives it has the advantage of reducing development time and costs. Unfortunately, this advantage is offset by the impact such an approach has on overall program structure. For example, one of EPA's design objectives was the development of a program of modular design to allow removal/replacement of various submodels. It is difficult to meet this objective when using large portions of existing software that may not have been developed with this objective in mind. The impact of this decision on the program structure in general and modularity in particular are discussed in detail in Section 2.2.3.

Figure 2-4 presents the overall program structure for PRESTO. It can be seen that the code is organized into recurrent or non-recurrent loops primarily on the basis of time. The main subroutine controls the program operation containing calls to all major subroutine modules. The first routine called is SOURCE which serves to read input data including both control information and technical data. The technical data includes information describing the properties of the cap, trench, aquifer, atmosphere, ground surface, food chain, uptake and nuclide inventory.



PROGRAM CONTROL
CALCULATION OF RESIDUAL ACTIVITIES
BASIN HEALTH IMPACTS

INPUT SITE/ENVIRONMENTAL DATA

UNIT SOURCE ATMOSPHERIC TRANSPORT

COVER INFILTRATION

COVER EROSION RATE

DOSE AND RISK CALCULATION

DOSE AND RISK CALCULATION

TRENCH WATER BALANCE

LEACHING

GROUNDWATER TRANSPORT

SURFACE SOIL CONCENTRATIONS

RESUSPENSION

DEPOSITION VIA IRRIGATION DURING YEAR

ATMOSPHERIC DEPOSITION DURING YEAR

HUMAN UPTAKE DURING YEAR

ANNUAL SUMMARY REPORT

AVERAGE DEPOSITION VIA IRRIGATION

AVERAGE ATMOSPHERIC DEPOSITION

AVERAGE HUMAN UPTAKE

DOSE AND RISK CALCULATION

Figure 2-4 PRESTO Program Structure

The first set of calculations performed by PRESTO involves the determination of an atmospheric exposure and deposition rate based on a normalized source. This calculation is initiated by a call to the main atmospheric routine AIRTRM which subsequently issues calls to DPLT to calculate plume deposition and SIGMAZ to calculate vertical dispersion. Additional routines called by this portion of the code include SIMPUN which uses Simpsons rule to integrate the ground level centreline correction and YLAG which performs a Lagrangian interpolation of dispersion related parameters.

The second set of calculations performed by PRESTO determines an average annual infiltration rate based on monthly maximum day length, daily mean temperatures and hourly precipitation for a typical year. The infiltration calculation is controlled by INFIL which reads additional control parameters and the meteorological parameters identified above. ROUT is a subroutine called by INFIL that performs the bulk of the calculation, both by calling SOIL, to determine the relative amounts of soil moisture, and subsequently iterating to determine the relative contributions of all mechanisms.

PRESTO then proceeds to perform some initialization calculations for the groundwater transport routine which results in the calculation of non-dispersed travel times as well as the evaluation of the decay-dispersion correction factor for each radionuclide. These calculations are performed primarily in the main routine with successive calls to QUANC 8 and FCN. These subroutines are generic in nature and perform an integration of a user specified function over user specified limits.

Additional initialization is performed for the cap erosion calculation by calling ERORF. This routine calculates an annual average cap erosion rate based on the Universal Soil Loss Equation.

Prior to entering the recurrent time loop, the last initialization is performed by two separate calls to the DARTAB subroutine. The first of these calls serves to read DARTAB input variables consisting primarily of human risk data. The second call to DARTAB calculates nuclide - pathway specific dose commitments resulting from a normalized waste inventory (i.e., dose factors) which are used in subsequent dose calculations.

At this point, the program enters the recurrent time loop. It should be noted that the time step for this loop is fixed at one year and the loop is executed for a user specified number of times. The first routine called within this loop is TRENCH which calculates the water balance in the trench based on volume in place, infiltration, (both into and out of the trench) and overflow. TRENCH uses a function known as CAP to calculate the integrity of the cap.

While within the time loop, the program executes two nuclide loops. The first of these loops calculates the movement of each radionuclide through the hydrologic pathway. These calculations commence with a call to LEACH to determine what fraction of the waste inventory is available for removal by leaching/dissolution as well as the quantity leaving the trench both through the bottom and as overflow. The flux leaving the bottom of the trench is used by VERHOR to calculate the concentration reaching the irrigation/drinking water well. The radionuclides overflowing the trench get added to an active soil zone on surface which contains whatever radionuclides may have originated from spillage. These radionuclides are subsequently removed by surface runoff to the stream (through SURSOL) or atmospheric suspension (SUSPND). The last calculation of the first nuclide loop is to update the mass of radionuclides present in both the trench and contaminated active soil zone.

The second nuclide loop within the time loop calculates the radionuclide accumulation in foodstuffs due to atmospheric deposition (FOODA) and irrigation water (IRRIGA) and the human exposure resulting from ingestion and inhalation (HUMEXA). At user specified times (IDELT) annual organ dose summary tables (via DARTAB) and annual transport summaries are printed (via OUT). This is the end of the main time loop.

Additional functions performed after the termination of the recurrent time loop include outputing a transport summary (via OUT) and dose and health calculations (via DARTAB) for the year of maximum dose. The dose and health calculations are either abbreviated (activated by setting POP = 1) or the comprehensive DARTAB suite. If the population is greater than one, PRESTO will go on to perform average dose and human health calculations over a user specified time period of interest. If average calculations are performed, calls are made to subroutines FOOD, IRRIG, and HUMEX for each nuclide. These routines perform analogous functions to FOODA, IRRIGA and HUMEXA for the annual calculations. A full suite of DARTAB calculations are then performed for the average exposures. This is the last set of calculations performed by PRESTO-CPG.

Appendix C contains EPA's descriptions of the various routines of PRESTO.

2.2.3 Extent of Modularity

One of EPA's design objectives in the development of PRESTO was the use of a modular design to allow the removal and/or insertion of an alternate submodel. AECB has also specified that modularity is a necessary requirement of their systems model. Unfortunately in spite of its stated design objective, PRESTO is not as modular as it could be, and certainly the replacement and/or addition of modules would require extensive interface programming.

Ideally modules should be totally independent of one another with a minimum number of variables being transferred between modules. All I/O should be contained within their respective modules to allow for the variation in input parameters that will exist between different submodels of the same pathway. The main routine should perform only program control (i.e., no calculations just calling of appropriate subroutines) and only key variables (such as concentrations at specific locations) should be transferred between modules.

PRESTO as it currently exists does not comply completely with the above criteria. For example, the majority of the input of PRESTO is read in a single routine (SOURCE) with smaller amounts read in INFIL and DARTAB. Because of this, the number of variables passed back and forth between the modules and the control portion of the program is significantly more than if the program were truly modular. In addition, PRESTO performs calculations in its main routine. These calculations are highly specific to the groundwater transport model currently employed by PRESTO and include the determination of a dispersion-decay correction factor for both vertical and horizontal transport regions. Obviously if this model were replaced by another transport model, these calculations would have to be removed in addition to subroutines such as VERHOR.

PRESTO is modular to the extent that specific routines are largely used to perform specific functions. For example, AIRTRM performs the majority of the air transport calculations while VERHOR calculates groundwater transport fluxes.

2.2.4 Level of Configuration Control

Configuration control is a software engineering term used to describe the level of consistency between various software components. This would include ensuring that the version of subroutines are consistent

with that of the main program and that the entire development history of the program is traceable. The current version of PRESTO contains or was subject to virtually no configuration control.

2.2.5 Quality Assurance

EPA currently has no official software quality assurance (QA) program in place other than a requirement to conduct a peer review of the final product. PRESTO has been subjected to such a review and a list of the panel members and findings is contained in Appendix D. In general, most of the criticisms voiced by the Peer Review Panel dealt with either the scope of PRESTO (e.g., additional scenarios that should be considered) or the validity of the approaches contained in the PRESTO program. Based on the results of the peer review, a number of actions were initiated (e.g., revisions to PRESTO). The exact nature of these actions is also presented in Appendix D.

It should be noted that Quality Assurance programs typically are comprised of a number of aspects such as:

- Performance Specifications;
- Design Specifications;
- Code Writing/Modification Procedures (e.g., baselining, version numbers);
- Testing (verification and validation);
- Audits;
- Documentation Procedures.

As indicated, EPA has no formal software quality assurance program in place. This fact is evidenced by the lack of such things as version numbers and creation dates for the program source. PRESTO has been subject to some level of QA in addition to the Peer Review Panel. This includes a QA audit performed by an independent consulting team as well as various verification tests performed on submodels of PRESTO prior to

their incorporation in PRESTO. The level of testing to which PRESTO has been subjected is discussed in a separate section on verification and validation.

The QA audit of PRESTO considered only the coding of the equations and the logic presented in the documentation and computer code excluding DARTAB and its associated subroutines. The audit involved checking the coding of equations, verifying results (by comparison with hand calculations), comparing the logic flow with that contained in the documentation, and verifying the transfer of variables between subroutines. The audit discovered a number of problems associated with unit conversions and material balance calculations. The modifications to correct the problems identified by the audit did not require major changes to either the code or its logic.

2.2.6 Verification and Validation History

While verification and validation are typically elements of any QA program, the absence of such a program does not preclude the existence of verification and validation testing. Several PRESTO submodels were subjected to testing independently of and prior to their incorporation in PRESTO. These tests, together with those performed as part of the QA audit, represent all of the testing to which PRESTO has been subjected.

It should be noted that in this report the term "QA" is used to refer to all possible components of quality assurance (e.g., verification and validation testing) regardless of whether they are elements of an official QA program. It should also be noted that in this report "verification" is used in the context of a procedure for establishing whether a piece of software meets its established design objectives (e.g., a program correctly solves a partial differential equation). Verification is not to be confused with "validation" the procedure

designed to ensure that specific performance objectives are met (i.e., a specific model adequately represents the real-world process for which it was intended).

Only a portion of the submodels contained within PRESTO have had some form of QA applied prior to their incorporation into PRESTO. Those portions of PRESTO that were subject to some form of prior testing include the INFIL and VERHOR submodels.

The INFIL submodel is used by PRESTO to determine the infiltration occurring through the trench cap. This model was originally developed by Hung (1983) and was tested by comparing the results to specific simulations to those obtained by other models. The model was intended to represent three conditions:

1. Gravity drainage without evaporation;
2. Steady state evaporation;
3. Vapor phase transport.

The first of these conditions was simulated and compared to the results of study conducted by Hillel and van Bavel (1976). While the comparison indicated that the time variation of flux was not duplicated exactly the agreement was generally close (within a few percentages) and the cumulative water agreed quite well. Because the infiltration model of PRESTO is intended to simulate average conditions over a one year period it was felt the model performance was adequate. The second condition identified above was simulated and compared to results obtained by Ripple et al. (1972). For this case, agreement between the two sets of model results was good. No data could be found by Hung (1983) to test the third condition identified and, although the model simulations follow the general trend described by Philip (1974), this aspect of the module should be regarded as untested. Fortunately from the standpoint of overall model realism the contribution of this component to the infiltration process is likely small.

The VERHOR submodel of PRESTO represents the saturated groundwater transport process. The model is based on an approximate solution to the convection-dispersion equation and makes use of a correction factor to account for dispersion and radioactive decay. Hung (1981) used an exact solution to the convection-dispersion equation to compare the accuracy of his approach. Hung (1981) concluded that his model performed adequately in all aspects for relatively long-lived nuclides but for relatively short lived nuclides over-estimated the lag-time associated with the arrival of the peak concentration. The magnitude and total contaminant discharge was the same in all cases. Based on these arguments, Hung (1981) concluded that his groundwater transport model could be integrated into the health effects assessment model without introducing any significant error.

The verification tests performed as part of the QA audit involved performing hand calculations to evaluate various components of PRESTO. These components included calculations for evaporation, erosion, water balance, infiltration, groundwater transport, surface water concentration, well withdrawal rates, suspension factors, atmospheric concentrations and nuclide concentrations in milk. Of these calculations only the atmospheric concentrations showed any discrepancy. These calculations initiated subsequent code changes for this submodel.

3. ABILITY TO MEET AECB REQUIREMENTS

The specific user requirements of AECB personnel are outlined in Section 1.2. This Chapter assesses the ability of the existing PRESTO program to meet these requirements. Because PRESTO-CPG contains all the features of DEEP and POP versions and in addition is the only one that performs dose calculations for the maximum exposed individual this assessment has been performed on the CPG version.

AECB requirements have been separated into two classes, those regarding technical capability and those pertaining to user oriented features. This distinction is not meant to distinguish between the priority of the requirement and merely represents a convenient way of grouping the user requirements.

3.1 Technical Capability

3.1.1 Dose Calculations over Time and Space

In order for AECB to evaluate a shallow land burial facility for radioactive waste the ability of such a waste disposal facility to meet AECB guidelines will have to be ascertained. This will necessitate the calculation of the maximum annual individual dose to members of the general public as well as a collective population dose for evaluation of the ALARA (As Low As Reasonably Achievable) objective.

PRESTO-CPG does calculate the maximum annual dose to an individual that resides at any user specified location. This dose is calculated for up to eleven organs including thyroid, red bone marrow, liver, skin, gonads, pancreas, kidney, breast, pulmonary, stomach and intestinal wall. A series of user supplied weighting factors is used to convert the organ doses to a total body dose. A collective population dose may also be calculated by PRESTO, however, it should be noted that because

population is considered to reside at one specific location this value is numerically equivalent to the product of the individual dose and the population. As outlined in Appendix B to obtain a collective dose for a site having different population centres would require multiple PRESTO runs. PRESTO is also capable of calculating the average dose over a user specified time span.

3.1.2 Simulate all Pathways

Before discussing the omission of pathways, it is appropriate to discuss the validity of the models used to simulate the pathways that are considered and in particular their suitability to Canadian conditions. It should be re-emphasized that PRESTO is a systems model and as such is intended to simulate the radionuclide migration through a variety of pathways. For this reason, the treatment of the processes/mechanisms within PRESTO may be viewed by some as simplistic. It should be remembered that PRESTO, like most systems models, is intended to be supported by a suite of single purpose models each capable of addressing a single portion of the exposure route in greater detail.

The treatment of the hydrologic pathway is in general acceptable with the majority of relevant mechanisms considered. Greater flexibility could be added if a groundwater contribution to the local stream were considered. However, because all eventual water uses (e.g., human consumption, livestock watering, irrigation) are comprised of a user specified mix of surface and groundwater the ability to have such a contribution is not essential. Another area where the inclusion of an additional mechanism may be of use is removal of radionuclides by sediment within the surface water body. A number of relatively easy and straight forward ways of incorporating removal of radionuclides by sediment exist. These include the use of a removal fraction or the use of a chemical equilibria compartment model. It must be recognized that a high degree of uncertainty surrounds sediment related behavior in surface water systems. In view of the current state-of-the-art with

regards to quantifying sediment effects in surface water bodies it is questionable whether the need to incorporate such effects is worthwhile. The same statement can be made regarding the treatment of cap erosion in PRESTO. Although the universal soil loss equation has been the subject of much criticism, there does not exist a better alternative having comparable level of sophistication.

The fundamental air transport model employed by PRESTO, a Gaussian plume model using dispersion parameters by Pasquill (1976), is widely accepted in the scientific community and is adequate to perform the calculations for which it is intended. The model should incorporate a mechanism to represent washout, with the radionuclides removed added to the soil surface. This could be accomplished by the use of a wet deposition coefficient such as that of McMahan and Denison (1979). The source term characterization is adequate in its treatment of soil contamination and suspension of contaminated particulates. It does make a fairly significant omission in the fact that it ignores the contribution of gaseous radionuclides. The presence of radon gas due to the relatively large percentage of radium 226 in most Canadian waste inventories is an example. The generation of radon within the trench, its diffusion through the overlying cap and overburden and resulting flux to the atmosphere will have to be considered for the majority of Canadian land burial facilities. This capability currently does not exist in PRESTO.

The approach used by PRESTO to estimate radionuclide concentrations in foodstuffs and the resulting dose to man is adequate for the evaluation of those foods for which it was intended. The model does not however consider such foodstuffs as fish and game, the inclusion of which is essential to estimate the impact under Canadian conditions. Another dose contributor that is not considered by PRESTO is the water immersion dose from swimming although this may be a conservative assumption depending on the relative amounts of activity present in the water versus that available on land.

With the exception of the mechanisms/pathways identified above, PRESTO should be capable of simulating Canadian conditions. There is sufficient flexibility within PRESTO to simulate typical Canadian waste inventories and dietary considerations. Canadian climatic conditions should also not pose a problem since snow accumulation and melting effects are considered within PRESTO. One small area where climatic effects are not considered and possibly should be is the shielding effect on surface exposure due to snow cover. The shielding properties of snow should be evaluated and could easily be incorporated in the surface exposure calculation as a reduction factor.

3.1.3 User Selectable Pathways

PRESTO currently does not allow the user to explicitly select the pathways to be considered. It is possible to virtually eliminate the contribution of various pathways by assigning specific values to parameters describing the mechanisms/processes present in the model. For example, the groundwater pathway can be overidden by using an unrealistically low value of hydraulic conductivity. Similarly, the runoff component of local stream contamination can be eliminated by setting the average land surface slope to zero, while atmospheric transport can be overidden by setting both the mechanical and time dependent suspension factors to zero or by setting the normalized radionuclide concentration to a number approaching zero. The contribution of contaminated surface water and groundwater to all of the possible surface water uses are calculated from user specified fractions and therefore can easily be removed from consideration.

3.1.4 Deterministic and Probabilistic Capability

PRESTO is currently solely a deterministic model having virtually no probablistic aspects associated with it. Obviously, in this capacity, PRESTO does not meet AECB requirements.

3.1.5 Miscellaneous

A number of additional capabilities required by AECB include:

- ability to evaluate different facility configurations (e.g., capped or uncapped, lined or unlined; shallow landfill, deep cavern);
- ability to specify dimensions and material properties for the facility (e.g., cap permeability and thickness, inventory);
- ability to incorporate the effect of up to three dimensions even if they are not considered explicitly;
- ability to specify simulation time period and time step.

PRESTO-CPG does have the capability of simulating a number of different facility configurations including shallow land burial, deep well injection, hydrofracturing and mined (cavern) disposal. Although the facility configuration may be selected explicitly, the features of the facility cannot be chosen as easily. For example, the model does not have an input parameter to decide whether the facility is capped or uncapped. However by specifying 100% failure of the cap from time zero, this effect can be simulated. Similarly, the existence of a liner is not determined by an input parameter, in fact the presence of a liner is not considered in PRESTO at all. However, it is possible to simulate the effect of a liner by modifying the permeability of the unsaturated zone underlying the trench/landfill. Transport within this zone will be one-dimensional with flow directed vertically downwards. All that is required to incorporate the effect of a liner is to use a hydraulic conductivity value that represents a weighted average of the liner and underlying host soil based on the relative thickness of each layer.

PRESTO has sufficient flexibility to allow the user to input such facility specific data as cap thickness and permeability, trench dimensions (depth, area) and waste inventory (up to 40 nuclides with their own solubilities, distribution coefficient, half lives). There are some instances, such as the trench liner identified above, where the parameter or feature is not considered explicitly although its effect can be incorporated.

Virtually all of the processes used within PRESTO have features that account for the effects of additional dimensions. In some cases, such as compartment models, this effect is included through the physical size of the compartment. Examples of this approach are the active soil zone and surface water models. The Gaussian plume model used for simulating atmospheric transport includes three-dimensional effects by virtue of its horizontal and vertical dispersion parameters applied along the plume centreline. The groundwater transport model also includes multidimensional effects by virtue of an aquifer thickness and dispersion angle. It should be re-emphasized that PRESTO is a systems model and should be supported by a suite of more sophisticated/detailed models. The concept of trying to use a multi-dimensional (possibly numerical) model to simulate one of the pathways should not be considered for a variety of reasons, including execution time, possible errors arising from space/time truncation, and memory limitations.

PRESTO does allow the user to specify the time period of interest including a lag time. For a variety of reasons however, it does not allow the user to vary the time step size. The main arguments in support of a fixed time step include:

- the time step is merely an averaging period not a numerical finite difference time interval;

- the logic within the code uses a yearly time step with seasonal variations incorporated into an average year. Significantly smaller (hourly) timesteps are used to calculate hydrologic processes over this time period;

- a time step larger in size than one year renders the calculation of an annual dose more difficult;

- a fixed time step (especially of unity) is easier to incorporate than a variable time step.

3.2 Necessary Features

3.2.1 User Friendly Input

PRESTO currently operates in a batch mode and consequently the onus is on the user to create the data input file in accordance with the format listed in the user manual. PRESTO is written in FORTRAN IV and therefore the user should be familiar with I, E, F and character format statements as well as NAMELIST read statements. The user is also responsible for creating and attaching a file containing dosimetric and health effects data. This file is generated by another program, RADRISK, in a format compatible with the input required by PRESTO.

PRESTO does echo the input data as read in and also typically prints variable values after they are read in. Virtually no checks are performed on input variables to see if they are within a feasible/credible range. One exception to this is a check performed to see if dose and risk factors are read in for all nuclides and organs. A limited number of input parameters have default values associated with them.

In summary, PRESTO is not very user friendly and relies upon the user to be computer literate.

3.2.2 User Controlled Output

PRESTO provides the user with very limited control over the type and quantity of output during the simulation. An input parameter known as IDELT will control the frequency of output of annual summary tables while a complete set of output tables by organ, nuclide and pathway is given for that year corresponding to the maximum year. To obtain this information at other user specified times would require the inputing of additional control variables and logical tests prior to the calling of the subroutine. For a purely deterministic run such limited control is probably adequate; however, for a probabilistic mode in which the results of hundreds of simulations will have to be presented such limited output control would not be acceptable.

3.2.3 Modularity

The extent of modularity of the PRESTO program is discussed in Section 2.2.3. As indicated therein, the code is not modular to the extent that would easily allow removal of submodels and insertion/addition of new submodels. This is due in large part to the presence of methodology specific calculations in the main routine, transfer of non-essential variables between routines and the existence of the majority of the input statements in a single routine.

3.2.4 Performance on HP1000

All software is subject to certain constraints imposed by the hardware on which the program must run. These constraints primarily include restrictions on physical program size imposed by central and virtual memory limitations and execution speed or turnaround.

Architectual considerations on the HP1000 require that large programs undergo a segmentation procedure. Although segmentation will be a required step in installing PRESTO on the HP1000, the availability of automated segmenting tools will assist the process.

The other area of concern is the turnaround time for a run. Turnaround time is distinct from execution (CP) time since on multi-user (tasking) systems execution time does not usually correspond to actual time. To assess the likely turnaround time on AECB's HP1000, PRESTO was set up compiled and run on an IBM-AT since a comparison between these two machines had been made (J. VanZettan, 1986). It was found that for a reduced size problem (1000 years and 10 nuclides) PRESTO required 9 minutes to execute on the IBM-AT indicating that 4.5 minutes of execution time would be required for a similar problem on the HP1000. Because the HP1000 supports up to eight users, actual turnaround time could be considerably longer. For a straight forward deterministic run, such a turnaround time would not be a significant deterrent to the execution of PRESTO. However for a probabilistic sampling procedure which would require hundreds or possibly thousands of simulations, such a turnaround time has more significant implications.

3.2.5 Self-Teaching Curriculum

Currently no formal self-teaching curriculum or tutorial exists for PRESTO. A number (more specifically three) of data sets exist that could be used as sample problems but the basis for the parameter selection is not discussed.

3.2.6 Restart Capability

Restart capability is a term used to describe the ability to continue a previously terminated simulation from either the middle or end of the run. Typically this involves writing out (or dumping) the entire memory at an intermediate point in the execution. A few control parameters are used to identify the restart run so as to avoid initialization tasks and proceed instead with the reading of the restart record. Restart capability is most useful in programs having extremely long execution times and numerous time steps. In the case of PRESTO (whose execution time is on the order of minutes), restart

capability would not be required in a deterministic capacity. For a probablistic sampling method however, the ability to perform additional simulations would be very beneficial. This would require as a minimum the ability to preserve the probability distribution functions for the input variables as well as the output values resulting from all the simulations performed to date.

3.2.7 Execution Error Messages

Execution errors basically consist of those associated with arithmetic operations (e.g., division by zero, arithmetic indefinites) or the evaluation of functions (argument out of range; overflow/underflow). In order to assist the user in identifying such occurences, it is necessary to evaluate and test the argument (or possibly individual components) and to print out corresponding warning messages identifying the location and possible source of the problem. Unfortunately although such messages are useful in debugging data sets and assisting people to become familiar with the program, there are certain disadvantages associated with such diagnostics, for example, increased run time and program size as well as the cost of incorporating such checks initially. PRESTO currently performs virtually no execution error checking and therefore fails to meet AECB requirements in this area.

3.2.8 Verified and Validated Program

One of AECB's requirements is that their systems model be fully verified and validated. The existing level of testing to which PRESTO has been subjected does not satisfy this requirement. However, it is conceivable that such a program could never be fully validated given the lack of suitable test data. Also due to the absence of any internal AECB QA, it is difficult to assess the ramifications associated with the shortcomings of this requirement.

3.3 Summary

While this section is meant to summarize those requirements of AECB that are not fulfilled by PRESTO, it is perhaps worthwhile to also point out those areas that are satisfied. For example, PRESTO does simulate the majority of pathways that could exist for a variety of waste disposal configurations and, in general, it does so using models that, while not overly sophisticated, are scientifically sound or represent the best available technology. Few "off the shelf" models could be expected to satisfy all of the diverse user requirements of a body like AECB and the cost of developing such a program from the beginning would be significant.

The major non-compliances of PRESTO with respect to AECB requirements therefore include:

1. Lack of: radon diffusion/inhalation pathway; fish and game consumption dose; water immersion dose; washout mechanism in atmospheric transport; sediment radionuclide interaction; shielding due to snow; groundwater contribution to surface water;

2. Pathway selection is not explicit but may be accomplished by variable (parameter) assignment;

3. PRESTO is completely deterministic having no probabilistic statistical aspects;

4. Time step is fixed and liner effects are not explicit;

5. Batch mode operation with limited validity checks; (program cannot be considered user friendly);

6. Extent of modularity does not allow for easy removal and addition/replacement of submodels;

7. Turnaround time of the order of five minutes;

8. Code documentation could be improved;

9. Code has been subject to some verification although only limited validation has been performed;

10. Only three sample data sets exist;

11. No restart capability exists, although such capability is only required for probabilistic capability;

12. The limited output control is adequate for deterministic applications but would require improvements for probabilistic modeling;

13. No execution error checks are performed.

4. ACTIVITIES TO MEET AECB REQUIREMENTS

In order to provide AECB with the capability it requires, a number of modifications to the existing program as well as the development of new supporting software (e.g., pre and post processing) and documentation will be required. It was originally hoped that such modifications could be accomodated without modifying PRESTO itself (other than conversion, I/O). However in view of the magnitude of the required changes necessitated by modularity changes, additional pathways, time step implementation and turnaround time, such a goal is unrealistic. In view of this, it must be recognized that a quality assurance program must be implemented to ensure the integrity of the developed software.

The following sections outline recommended action to provide AECB with a code capable of fulfilling their user requirements. In most cases, a recommended approach is proposed based on its compatability with other AECB requirements and the existing software.

All software development should include the following general activities:

1. write performance specifications - general objectives;
2. write design specifications
   - suitability of existing program functions;
   - integration into existing routines;
   - identify possible conflicts
3. Implement and test
4. Document

These general tasks pertain to all proposed software development activities described in the following sections. Specific issues that should be considered for each of these tasks have also been identified.

4.1 Additional Pathways/Mechanisms

In order to meet AECB's requirement of realistically simulating all potential pathways, a number of mechanisms/pathways should be added to PRESTO and a number of mechanisms should be evaluated and based on this evaluation either added or discarded from the systems model package. These features include:

- radon gas effects;
- fish and game consumption;
- water immersion dose;
- washout for atmospheric pathway;
- sediment effects for surface water pathway;
- snow shielding effects;
- groundwater contribution to local surface water.

Each of these additional mechanisms/pathways together with proposed methods of incorporating them into the existing software configuration are described separately in the following sections.

4.1.1 Radon Gas Effects

Due to the potentially large volume of radium within Canadian waste inventories, the inhalation of radon gas (a short lived daughter product) may result in a significant dose contribution. To incorporate this pathway into the existing PRESTO model, the following general issues should be considered:

1. Performance related:
   i. Mechanisms - e.g., diffusion, convection decay through cap; atmospheric transport; inhalation dose

   ii. Conditions - time period, transient versus steady state, dimensionality

2. Design related:

Possible approaches - e.g., empirical, analytical, numerical

Performance specifications will have to be written to identify the objectives of the intended code development/modification. For the case of radon gas, this will entail identifying those mechanisms which control the release and migration of radon gas and evaluating the conditions which the model is intended to simulate. In this particular case, it is most likely that diffusion of radon through the cap will be the dominant mechanism with convective effects being negligable. In addition to radon diffusion through the cap which would have to be considered under the normal operation scenario, the dose arising from inhalation of radon and its daughters in a basement would have to be considered for the resident intruder scenario. Given the relatively short half life of radon 222, it is fairly certain that radioactive decay will have to be considered. The conditions under which these mechanisms need to be evaluated may require further investigation before being defined. A one-dimensional solution to the diffusion equation will in most cases be adequate; however, it is uncertain whether a steady state solution would be sufficient.

Having defined performance objectives the next step is to assess the best method of achieving these objectives. For example, should radon gas diffusion through the trench cap be incorporated as an analytical solution such as those proposed by Rogers et al. (1980) and Freeman and Hartley (1984) or a numerical solution (Mayer et al., 1981). Obviously, these methods will have to be evaluated both in the context of their ability to solve the radon gas diffusion problem and their consistency with overall system model objectives.

The diffusion of gas through a partially saturated media is just one component of the radon inhalation pathway. In addition, larger scale convective-dispersive transport may have to be considered as well the

dose resulting from the inhalation of the gas itself. Although particulate transport is currently handled through the use of Gaussian plume model, it is questionable whether the same model could be used for radon gas. This is due to the fact that radioactive decay is ignored in the model, an aspect which is not overly restrictive in most cases but, owing to the relatively short half lives of radon and its associated daughter products, may pose a difficulty. The existing Gaussian plume model would also have to be modified to by-pass the plume reduction due to dry deposition, a process which should not be considered for gaseous radionuclides. The short half lives of radon and its daughters may also cause a problem in the use of the existing dose calculation algorithm. Although the original version of DARTAB did evaluate a dose resulting from radon and its daughters (using an approach based on working levels) because PRESTO did not consider radon gas effects, this portion of the code has been removed (via commenting) or by-passed. It is therefore uncertain as to whether the original methodology used would be compatible with the performance objectives and furthermore whether the existing version of DARTAB within PRESTO could be reverted to its original capability. These items will have to be evaluated as part of any attempt to incorporate radon gas effects.

Once performance specifications have been established and an approach has been selected then a method of integrating the additional requirements into the existing software must be devised. This will involve evaluating I/O requirements, additional subroutines and interfaces, and designing the appropriate software. At this point, areas of possible conflict (e.g., memory allocation) should be indentified and flagged for subsequent testing.

The next steps are the implementation (coding) and testing. These two activities typically run concurrently since software is usually verified as part of the development process. Both the development and execution of verification tests will be conducted in this activity. In addition, a validation test should be constructed

(provided sufficient data exists) to ensure the model adequately represents the physical process. A preliminary form of validation should also take place during the evaluation of possible approaches (item 2(i) above) but this is generally more a review of reported validation.

4.1.2 Fish and Game Consumption

This requirement is necessitated primarily by the possible need to evaluate land burial facilities in remote areas where a significant portion of the resident's diet consists of wildlife. As with the radon gas pathway, the following general issues should be considered.

1. Performance related:
   i. Mechanisms - bioaccumulation, water, sediment concentrations
   ii. Conditions - marine, fresh; types of game; equilibrium

2. Design related:
   Suitability of existing program functions - surface water concentration calculation

It is anticipated that the dose factor approach used within PRESTO will be adequate to represent the ingestion dose from game and fish. Fish concentrations will be a function of surface water concentrations creating the need for accurate determination of groundwater contribution to surface water (an aspect which is currently not considered by PRESTO). Assuming the primary game animals are herbivores, the approach utilized by PRESTO to calculate the dose resulting from the ingestion of contaminated beef can also be used for game animals.

A moderate level of difficulty is anticipated with the integration of new features into the existing software. The major source of difficulty is associated with the accurate determination of surface water concentrations (i.e., the addition of a groundwater component). PRESTO currently calculates a single set of decay-dispersion factors initially and uses them repetitively thereafter. It may be necessary to define an additional array to represent the extra pathlength (to the surface water body). The inclusion of the remainder of this pathway would be relatively straight forward. Integration into the existing code would require only I/O and other minor coding changes. Verification testing should also be relatively easy to accomplish although validation may be impossible to perform due to insufficient data.

4.1.3 Water Exposure Dose

The external dose resulting from either immersion into a contaminated water body or proximity to such a water body is not considered by PRESTO. As with the modifications outlined previously, the following general issues should be considered.

1. Performance related:
   Mechanisms - immersion, dose due to proximity

2. Design related:
   i. Evaluate possible approaches - dose factor
   ii. Suitability of existing program functions - e.g., exposure calculation

The inclusion of both types of dose resulting from surface water bodies should be relatively straight forward. It is anticipated that both of these exposures could be handled through the use of dose factors and exposure times. As with the fish ingestion calculation, these calculations will require the accurate determination of surface water

concentrations (necessitating the addition of groundwater discharge component). The necessary code changes should be relatively minor being mostly I/O or the addition of additional exposure contribution calculation. As was the case for fish/game ingestion, dose verification should be straight forward although validation may be more difficult.

4.1.4 Washout for Atmospheric Pathway

Washout of airborne contaminants is a process which is currently not considered in PRESTO. This process may alter plume and ground surface concentrations significantly and as a result should be incorporated into the model. The general issues to be considered in incorporating this feature in PRESTO are:

1. Performance related:
   - i. Mechanisms - removal from plume, add to soil surface
   - ii. Conditions - annual average

2. Design related:
   Evaluate possible approaches - e.g., wet deposition coefficient

The addition of this capability through the incorporation of a wet deposition coefficient would involve reducing air borne concentrations and adding the removed mass to the soil surface. The removal of radionuclides may be a function of the state of the radionuclide (e.g., gaseous or particulate) a consideration which should be evaluated. The addition of this capability to PRESTO will require few software modifications and no use of existing program functions making it relatively straight forward to integrate into the existing code. Verification of the coding should be capable by hand calculation while validation of the feature will be dependent on availability of data.

4.1.5 Surface Water Sediment Effects

The addition of surface water sediment effects into PRESTO may represent an important sink for dissolved radionuclides. To incorporate this mechanism the following general issues should be considered:

1. Performance related:
   i. Mechanisms - e.g., partitioning
   ii. Conditions - e.g., equilibrium

2. Design related:
   i. Evaluate possible approaches - distribution coefficient, kinetic
   ii. Suitability of existing program function - e.g., active soil zone

If the incorporation of sediment effects into PRESTO may be adequately represented by an equilibrium adsorption isotherm, it may be possible to use existing portions of PRESTO to simulate this function. The active soil zone above the trench uses a similar approach to simulate soil - radionuclide interaction. The existing software may require recoding because it currently is quite specific. Ideally a generic function that calculates the partioning between soil/sediment using water concentration, distribution coefficient and a finite soil/sediment volume is required. Verification testing of both the active soil and surface water sediment portions of the code would be required. Validation of this process may be difficult since in situ data is sparse although laboratory data is available.

4.1.6 Snow Shielding Effects

The impact that snow accumulation has upon external exposure dose from contaminated ground surface is a mechanism that currently does not exist in PRESTO. Because the climate in Canada is such that snow shielding effects may be significant this aspect should be investigated and incorporated. To incorporate such a feature, the general issues that must be considered are:

1. Performance related:
   - i. Mechanisms - exposure reduction
   - ii. Conditions - average annual

2. Design related:
   - i. Evaluate possible approaches - e.g., shielding factor
   - ii. Suitability of existing program functions - use exposure dose and meteorological portions, add new variables

The addition of an exposure reduction mechanism can most easily be incorporated as a shielding factor. This factor would represent the average reduction in dose due to snow in a given year and can be either included as an input variable or calculated in the infiltration routine which keeps track of snow accumulation throughout the average year. By calculating a time dependent shielding factor based on accumulated snow depth, the average annual shielding factor can be determined. Having obtained the average annual shielding factor, it would be used in the external dose calculation portion of the code as a reduction factor for both the normal and resident intruder scenarios but should only apply to the time spent outside. Integration of this capability within PRESTO would require the addition of input variables, the addition of an average shield factor calculation in the infiltration routine and the incorporation of the factor into the external dose calculation routine.

Verification of the average shielding factor determination and use could be accomplished through hand calculations. Validation testing would depend on the availability of suitable field data.

4.1.7 Groundwater Contribution to Surface Water

The need for accurate surface water concentrations may be required regardless of whether the dose from immersion or ingestion of contaminated fish is deemed a requirement. To incorporate this feature the major issues to be followed are:

1. Performance related:
   - i. Mechanisms - groundwater flow and transport
   - ii. Conditions - steady state flow, transient transport

2. Design issues:
   - i. Evaluate possible approaches - analytical; existing
   - ii. Integration into existing program - additional arrays

There are a number of ways of incorporating the groundwater contribution of radionuclides to surface water systems. The most logical way would be to make use of the existing groundwater transport model of PRESTO. This would still however, necessitate some modifications to account for the boundary conditions that exist between the local stream and the upstream reach (possibly the well location). In addition, the percentage of water in the aquifer that discharges to the stream would have to be estimated. To integrate such changes into PRESTO would require the addition of input variables (e.g., pathlength, groundwater velocity), another decay dispersion array and boundary condition (e.g., source) modifications.

The additional software could be verified through the use of a numerical solution to the convection dispersion equation. Success of validation efforts will depend largely on availability of data.

4.2 Interactive Input/Output Process

4.2.1 Data Input

To ensure that those AECB personnel who have little knowledge of, or familiarity with, computers can make use of PRESTO's capabilities, a user friendly pre-processor could be constructed to interface with the user. The pre-processor would be interactive, micro based and probably menu driven. In this way, the user could create new data sets or modify existing data sets by responding to prompts and menu selections. Ideally, the pre-processor would create a file in a format that is compatible with the input requirements of PRESTO, minimizing the need for extensive modifications to PRESTO itself. The user friendly input pre-processor would require consideration of the following issues:

1. Performance related:
   - e.g., input pre-processor to assist the creation of a PRESTO data set
   - create and edit
   - interactive (menu driven)
   - independent of PRESTO

2. Design related:
   - IBM-PC type target hardware
   - implementation language(s)
   - error checking/default values

The creation of performance and design specifications is an activity which should be carried out in conjunction with AECB personnel. The items listed above are merely examples of the things that should be considered and do not necessarily represent a recommended nor comprehensive list.

4.2.2 Post-Processing of Results

The need for post-processing of results would be greatest for the probabilistic capability scenario because of the vast quantity of output that could potentially be generated. This aspect is discussed in the section on the probabilistic capability (Section 4.3). There may be some need, even for purely deterministic simulations, to have the capability of graphically presenting the data in different ways. This would be especially true if the simulation period is quite long.

The following software development issues would be addressed:

1. Performance related
   - graphic representations (xy plots, histograms, curve fitting)
   - others as identified by AECB staff
   - hard copy requirements
   - labelling and titling

2. Design related
   - implementation language(s)
   - target hardware

4.3 Probabilistic Capability

There are considerable uncertainties associated with most of the input variables of a model like PRESTO when used to analyze a specific site. Many of these input variables may be relatively unimportant in the sense that the model output is not very sensitive to them. However, important input variables to which the model is known to be sensitive (e.g., distribution coefficients and waste leach rates) may also be subject to considerable uncertainties. Therefore, dose estimates obtained from the systems model may be subject to large uncertainties.

Any systems model used by AECB must be structured in such a way that input data uncertainties can be taken into account in a relatively convenient manner. There are several techniques available for addressing sensitivity and uncertainty analysis, including differential techniques, stochastic modeling and statistical sampling methods. Differential techniques are restricted to instances where model output is not a highly non-linear function of model input, which unfortunately is not the case for shallow disposal radioactive waste models. Stochastic models require significant development effort as well as considerable computer memory and run time. For these reasons and because PRESTO is currently a deterministic model, the use of sampling methods is the most feasible approach to uncertainty analysis. Although a number of sampling methodologies exist, it is recommended that only two be considered for inclusion into a probabilistic version of PRESTO namely Monte Carlo (MC) and Latin Hypercube (LHS) sampling. There are several reasons for this including:

1. A LHS sample of size one is equivalent to a single MC sample and hence most LHS sampling software can be easily adapted to provide a MC sampling capability;

2. Dual capacity provides verification capability;

3. LHS is more efficient than MC requiring 3 to 4 times less computer time to achieve the same level of accuracy;

4. Sensitivity to input variables can be assessed by calculating partial correlations on ranked data (for LHS).

This latter feature will simplify uncertainty and risk analysis by helping eliminate unimportant variables from consideration. Furthermore, this sensitivity analysis capability will help identify areas where better data are needed to reduce output uncertainty.

In addition to the features identified above, the sampling methodology must have the capability to account for correlations among input variables. The importance of input variable correlations on output variable distributions was discussed in a previous report (GTC, 1985).

As with the previous software development activities, the same general issues must be considered:

1. Performance related:
   - i. Sampling methodology with user specified pdf's
   - ii. Maximum turnaround time limit
   - iii. Correlations among input variables
   - iv. Sensitivity analysis

2. Design related:
   - i. Micro based pre-processor to generate pdf's
   - ii. Driver routine to perform sampling
   - iii. Probabilistic and deterministic
   - iv. Post-processing and graphical capability
   - v. Restart capability

The need for the features identified under performance specifications was discussed above. The design specifications identified herein are general and merely serve as a guideline to the type of activities that should be considered. A micro based pre-processor would allow faster generation of input pdf's and not adversely affect mainframe execution. The input pre-processor would be designed to either create new data sets or edit existing ones. The pre-processor could also be made user friendly (e.g., menu driven) to assist those not fully computer

literate. A driver program should be used to perform the sampling protocol on the main frame after creation of the input pdf's to free up the user and communication network. The probabilistic aspect should be capable of being overidden if a purely deterministic run is desired. This feature could also be easily be incorporated into a pre-processor program.

Due to the quantity of output likely to be generated by a probabilistic model, some post-processing of the simulation results will be essential. This post-processing should also be micro based since interactive graphical display of data (e.g., scatter plots, histograms, partial rank correlations, complementary cumulative distribution functions (CCDFs)) does not require mainframe resources.

The following discussion focusses on typical post-processing and graphical display techniques. They are not meant to be all-inclusive but merely represent a cross-section of the kinds of post-processing that should be considered.

Partial correlations are generally more useful than simple correlations since they show the correlation between two variables after the effects on variation due to the presence of other variables have been systematically eliminated. The top few variables can be interpreted as those contributing most to model uncertainty.

The CCDFs, histograms, and scatter diagrams are typical means of graphically displaying sets of results. Histograms serve as discrete representations of distribution functions. CCDFs are complements of the integrals of the distribution functions. Scatter diagrams can be used to show correlation patterns between variables.

A probabilistic model may require hours or even days of execution time. To avoid the loss of interim results due to system failure or incomplete convergence, it is desirable to provide the user with the

capability of restarting a simulation from an intermediate execution point. This can be accomplished by creating a file on the mainframe and periodically writing the entire memory to it.

Testing of the probabilistic aspects of the model is essential and may be accomplished either through the design of test cases having known outcome or by comparison of LHS and MC results.

4.4 Enhanced Modularity

The enhanced modularity activity arises from a combination of AECB's need to add and/or replace submodels and the current extent of modularity in PRESTO. In order to modify PRESTO to the extent required by AECB the same general software development issues should be addressed:

1. Performance related:
   - new submodels should be added or replaced in such a way so that a minimum amount of software modification is required;

2. Design specifications:
   - all input (and associated checking, echoing) to be contained in appropriate sub-model
   - minimum transfer of variables
   - main routine provides program control only
   - QA version numbers for main program and subprogram

The minimum required software changes needed to replace a submodel would ideally consist solely of changing a subroutine call. All software relating to variable input, error checking and echoing of input data should be contained within the module in which it is used. Only essential variables should be passed between program modules. This would include such essential information as concentrations at a specific location and time, control variables and unit numbers. Currently PRESTO is not modular to this extent. To achieve the

performance objectives stated above would specifically involve:

1. Removal of calculations from PRESTO mainprogram
2. Changing location of input reads (from source to appropriate routine)
3. Eliminating non-essential variable transfers through common blocks and argument list.

Obviously, the extent of such changes dictates the need for comprehensive QA procedures and in particular testing of the developed software. Whenever the transfer methodology between subprograms is altered the probability of introducing obscure errors increases significantly. Verification tests will have to be designed to ensure the intended variable transfers are conducted in accordance with original performance objectives.

4.5 Miscellaneous

The activities needed to fulfill the remaining user requirements of AECB that may not be met by PRESTO are discussed in this section. Briefly these requirements include:

- variable time step
- explicit provision of liner
- verified code and validated performance
- provision of a self teaching curriculum
- execution error messages
- explicit selection of pathway/mechanisms
- make hard programmed variables user selectable.

The variable time step is a requirement that is not currently available within PRESTO and would require substantial effort to incorporate. PRESTO is currently based on conditions (e.g., meteorological, infiltration rates, etc.) that are representative of a typical year. Seasonal dependence is incorporated initially through the calculation

of average annual conditions. To incorporate a variable time step would require substantial changes to the overall logic (since seasonal effects would have to be handled differently). In addition, the inclusion of a variable representing a time step has been omitted from many of the code equations (since it is assumed equal to one). Changing the time step would require recoding (and associated testing) of all relationships having a time step dependence.

A number of the AECB user requirements are not explicitly satisfied by PRESTO. These include such features as user selectable pathways, and liner properties. As mentioned previously (Chapter 3) pathways may be selected based on judicious selection of input variables while liner effects may be incorporated into the hydrogeologic properties of the vertical reach underlying the trench. Alternately these pathways may be incorporated explicitly into PRESTO through the modification of software. In the case of user selectable pathways/mechanisms this could be accomplished by the addition of control variables and the insertion of logical tests at strategic points within the code. Liner effects could be incorporated explicitly by adding a control variable to the input list. If the value of this variable is such that it indicates liner effects are to be considered then additional input variables, defining the thickness and permeability of the liner, would be read in. These variables would be used in the calculation of an equivalent hydraulic conductivity of the materials beneath the trench using a weighted averaging technique based on the relative thickness and permeabilities of the materials. The new equivalent hydraulic conductivity could be used in the existing PRESTO algorithm.

PRESTO and its components have been subjected to various levels of verification and validation. In view of the difficulty associated with obtaining test data (for the purpose of program validation) it is unlikely that complete validation of PRESTO is currently feasible. In light of this fact, together with the absence of any formal QA

requirement of AECB, it is difficult to define what additional testing of PRESTO should be required. Given the lack of a formal EPA QA program, it seems likely that at least comparison to hand calculations may be required.

As indicated previously no self teaching curriculum currently exists for PRESTO. Three sample problems are contained within the existing documentation but are not fully described. The creation of a self teaching curriculum should start with these sample problems but be more fully documented including justification for parameters. It must be recognized that the development of a self teaching curriculum is rather open ended and can be made as comprehensive as desired. Certainly demonstrative use of major program functions would be required.

PRESTO currently has only very limited run time diagnostics consisting of error checking of some input variables. Ideally run time diagnostics should include error checking on all input variables (ensuring that they are in a credible range) as well as checks on arguments prior to the execution of arithmetic operations. This will prevent such errors as division by zero, exponent over/under flow, arithmetic indefinites, etc. If a potential problem is found, a warning/error message should be printed indicating the likely source of the problem. While execution time diagnostics are beneficial in both learning how to use the program and initial debugging of data sets it must be recognized that such benefits extract a price on the overall code efficiency.

The vast majority of hard programmed variables (values) are used relatively few times and as factors. To enable these values to be user specified would require new variables to be defined through read statements and the associated values to be passed via common block or argument list to the routine in which it is to be used. Two exceptions

to this general classification of hard programmed variables are the fixed time step and sector angle. Both of these values have significant logic/data requirements associated with their selection. The ramifications associated with variable time step have been discussed above. A variable (or user specified) sector angle is probably unjustified because insufficient meteorolgical data will be available to justify the use of more than 16 grid sectors.

5. IMPLEMENTATION PLAN

5.1 Possible Scenarios

Due to the relatively broad range of activities needed to fulfill AECB requirements, the cost of implementation may be prohibitive. For this reason, a number of possible implementation plans have been desribed which, although not fulfilling all of the AECB requirements, do present a series of logical alternatives to AECB. This approach also provides AECB with some estimate of the marginal cost associated with the fulfillment of additional requirements. Four scenarios have been considered:

1. Installation of PRESTO on AECB's HP1000 and modifying to include additional pathways/mechanisms;

2. Scenario 1. with the addition of a user friendly interface;

3. Scenario 1. with probabilistic or deterministic capability;

4. Full capability version including all modification necessary to meet AECB requirements.

A proposed implementation plan for each of these scenarios is discussed in the following sections.

As indicated previously, it will not be feasible to incorporate the necessary requirements within PRESTO without modifying the original code. As a result, a substantial Quality Assurance program will have

to be followed for all aspects of software development. The procedural activities that should comprise such a program are discussed in detail in Section 5.2.

5.1.1 PRESTO and Additional Pathways

This scenario would consist of the following tasks:

1. Installing PRESTO on AECB's HP1000;
2. Documenting required changes (e.g., FORTRAN 77 conversion, system architecture dependent segmentation);
3. Testing (including development of test methodology and test cases);
4. Baselining;
5. For each proposed modification (i.e., pathway)
   i. writing performance specifications
   ii. writing design specifications
   iii. implementation and documentation
   iv. testing;
6. Baselining.

The installation of PRESTO onto AECB's HP1000 will require some conversion due to compiler and machine differences. This conversion will require modifications to such items as I/O (e.g., units used, namelist read statements), common blocks (those of varying size) and some program logic (e.g., transfers to the middle of a Do-loop). AECB's HP1000 system architecture will necessitate segmentation of the code. Due to the nature of these and other conversion/installation changes it is essential that an accurate record be maintained of all such changes. This will assist the software developers not only during the installation phase but subsequently (possibly many years hence) in the tracing of obscure program errors. Once the code has been installed upon the HP1000 it must be thoroughly tested to ensure the

installation process has not compromised the integrity of the code. This will essentially be a form of verification testing and could involve the development of test methodologies that might include:

1. Running test cases;
2. Memory, transfer tests;
3. Independent audits.

Having successfully completed the testing phase the next step would involve baselining. Baselining is a quality assurance term for a process that involves archiving a specific version of a computer program. Typically a unique quality assurance version number is assigned to the code and must be used in the running of subsequent data sets to ensure traceability of input, output and version. A master copy of the program is stored in a secure location on a "read only" tape, with backups created in accordance with the specification of the QA program. A baselined code is virtually always used as a starting point for further code development.

The level of detail pertaining to the performance and design specification tasks was indicated in Section 4 for each of the additional pathways (mechanisms). The actual order in which these pathways/mechanisms would be incorporated is, at this point, undecided. However, it must be recognized that certain modifications will overlap one another. For example, the determination of accurate groundwater contributions to surface water bodies is needed for the determination of fish concentrations and water immersion/exposure dose. Wet deposition in the atmospheric model may affect the radon gas model as well as the soil surface radionuclide concentrations. This latter aspect may affect the implementation of a sediment radionuclide model, if the active soil zone model is used for this purpose. The nature of these overlapping modifications emphasizes the need for a comprehensive verification testing component for the proposed modifications.

5.1.2 PRESTO, Additional Pathways and User Friendly Capability

Under this scenario the following tasks would be conducted:

1. All tasks discussed in Section 5.1.1;
2. For the user friendly input pre-processor
   i. writing performance specifications
   ii. writing design specifications
   iii. implementation and documentation
   iv. testing;
3. Baselining;
4. For the output post-processor
   i. writing performance specifications
   ii. writing design specifications
   iii. implementation and documentation
   iv. testing;
5. Baselining.

Examples of the activities contained in each of the software development tasks for the input pre-processor and output post-processor are contained in Sections 4.2.1 and 4.2.2, respectively. Although the development of the input pre-processor has been placed prior to that of the output post-processor, this need not be the case and development of these aspects may proceed independently of each other.

5.1.3 PRESTO, Additional Pathways and Probabilistic Capability

This scenario describes the activities required to install PRESTO on a computer, implement additional pathways and provide a probabilistic capability. The major tasks involved in this scenario are:

1. Evaluate streamlining of PRESTO;
2. Tasks discussed in Section 5.1.1;

3. Additional tasks discussed in Section 5.1.2 plus enhancements required to deal with input and output of pdfs.
4. For mainframe driver:
   i. writing performance specifications
   ii. writing design specifications
   iii. implementation and documentation
   iv. testing;
5. Baselining.

The first major task outlined above serves to evaluate the possibility that a modified version of PRESTO could be made to run at a speed necessary to perform hundreds (or possibly thousands) of simulations within a reasonable time period. PRESTO would require approximately 5 minutes of CP time on AECB's HP1000 to simulate 10 nuclides for 1,000 years. This time is prohibitively long from the standpoint of providing a probabilistic capability. However, PRESTO currently performs many calculations that are in excess of the requirements of AECB (e.g., risk analyses). It could be beneficial to examine how much faster PRESTO could be made to run by eliminating these unnecessary calculations. If such a streamlining of PRESTO was not sufficient to decrease simulation time to an acceptable level then AECB's only other alternative would be the acquisition of additional faster computing resources. The potential cost savings associated with such a streamlining operation would definitely justify its examination.

5.1.4 Full Capability Version

The following tasks comprise a possible implementation plan to meet all of AECB's stated requirements that are not fulfilled by the current version of PRESTO. This plan tacitly assumes that sufficient computer resources are available to meet turnaround requirements for a probabilistic routine.

1. Tasks identified in Section 5.1.1;
2. Additional tasks specified in Section 5.1.2;
3. Additional tasks specified in Section 5.1.3;
4. For each feature to be added (variable time step, explicit liner and pathway selection, execution diagnostics, enhanced modularity)
   i. writing performance specifications
   ii. writing design specifications
   iii. implementation and documention
   iv. testing;
5. Create self teaching curriculum;
6. Baselining.

Tasks 4 and 5 represent the incorporation of additional features such as variable time step, explicit pathway and liner selection, execution diagnostics, enhanced modularity and the development of a self teaching curriculum.

5.2 Quality Assurance Procedures

All proposed software development should be subject to a high level of quality assurance (QA) to ensure the developed code meets its design and peformance objectives. The QA program should contain guidelines not just for the testing of programs, but also define procedures to be followed in the development and implementation of the software. These items are discussed separately in the following sections.

5.2.1 Code Modification

The QA program that should be adhered to during the development and coding should comprise such elements as:

1. Documenting performance objectives;
2. Documenting design specifications;
3. Documenting both the additional coding required as well

as any changes/modifications required to existing software;

4. Verification and testing;
5. Baselining code and verification test results;
6. Audits.

Performance objectives are meant to describe the general capability of the proposed software. Design specifications detail the approach to be followed in achieving the performance objectives and include required software modifications. Both of these items as well as the actual software changes must be documented in accordance with the protocol of a QA program. The documentation procedure results in a formalization of the QA function and frequently forces the developer to spend more effort in the definition of his needs. Obviously, there are long term benefits associated with such a procedure. Part of the documentation procedure also involves the documenting of the code itself to identify the changes made. Both during and after software development, the program should be verified for its correctness (this aspect discussed in Section 5.2.2). Once it is established that the developed software performs satisfactorily, the code, together with its performance and design specifications and verified test cases is baselined. Baselining (or benchmarking) involves archiving the finished software product together with its associated documentation and assigning version numbers to all components. Audits are, as the name implies, an independent reivew to ensure compliance with QA procedures.

It is recognized that AECB currently has no formal QA program in place to govern the development/modification of scientific (modeling) software. The components identified above represent general items that should be considered in the development of software for PRESTO. It is recommended that such a set of QA procedures be formally adopted prior to the development of any software. QA is difficult to apply after the fact and, in the long run, the effort required to maintain a QA

qualified program is more than offset by reductions in development and debugging time, the increased confidence level in the code's performance, and the enhanced traceability of code evolution throughout the software lifecycle.

5.2.2 Verification and Testing

Verification and testing are elements of QA programs but due to their comprehensive nature have been discussed separately. Verification as used in this report is meant to represent the process of ensuring that the program is coded correctly. Validation on the other hand is a process to ensure the program meets its performance objectives. Verification involves much more than the execution and comparison of sample data sets. Proper verification should involve the construction of test cases to test out possible conflicts within the code. Ideally, the construction of test cases should also conform to QA procedures and involve the writing of test performance and test design specifications, documentation and baselining of results. Verification may be static (e.g., analyses of code structure) or dynamic (execution of test cases) with most QA programs having both components. In the case of PRESTO, verification should begin with individual modules, progress to groups of modules and then proceed to the integrated program.

5.3 Instruction

Regardless of the scenario selected, some level of instruction will be required to assist AECB personnel in learning PRESTO's capabilities as well as the features of possible interfaces. The level of instruction may be varied and will also be a function of the scenario selected. For example, Scenario 1 does not provide a user friendly interface and consequently the level of instruction required will be higher than for, say, Scenario 2. The features provided by the interface also will influence the level of instruction required. An input pre-processor for a probabilistic/determination simulator would require more explanation than a purely deterministic one.

The instruction task could involve the following activities:

1. Modifying existing documentation;
2. Creation of additional and better documented sample problems;
3. Creation of a demonstration simulation package;
4. Courses.

5.4 Hardware Considerations

A deterministic version of PRESTO could be expected to perform adequately (turnaround less than 1 hour) on AECB's HP1000. For a probabilistic (specifically sampling) methodology the existing computer resources of AECB would not provide reasonable performance. Given that a single deterministic run would take 10's of minutes, together with the existence of 50-75 input variables requiring pdf's (each requiring 10 simulations for LHS) anticipated turnaround time would be on the order of weeks. To achieve a turnaround time of the order of a day, AECB should consider the acquisition of a mini-computer with execution speeds at least an order of magnitude faster, something equivalent to a VAX 8300 series computer. To achieve turnaround on the order of an hour, the acquisition of a super mini-computer (VAX 8800 or its equivalent) would be required.

It should also be pointed out that although a deterministic version of PRESTO could execute on the HP1000, some consideration should be given to implementation on a micro computer (such as an IBM-PC/AT) if deterministic-only capability is considered. This would eliminate the need for alternate computing environments for pre- and post-processors and program execution. This would preclude the need for intermachine communications. Additional considerations for this scenario are provided in Appendix E.

6. LEVEL OF EFFORT

A few general statements can be made regarding the level of effort required to undertake the software development tasks necessitated by AECB user requirements.

First the level of effort required to adhere to a Quality Assurance Program is not insignificant and typically may be equal to 50 - 100% of the level of effort to develop the software. In the long run such an expenditure is cost-effective since it will serve to reduce development and debugging time. Costs can not be reduced by eliminating or downscaling this task since they result in cost increases elsewhere.

Secondly, the level of effort to perform various tasks may not be linear. The sum of the cost of performing two software modifications independently may not be the same if the two tasks were done concurrently. By selecting a number of likely scenarios such as undertaken in this study, such non-linearities may be taken into consideration.

Lastly, it must be recognized that a certain percentage of additional development cost may be required for a new developer to become familiar with PRESTO to the point of being able to incorporate the necessary software and design suitable test cases. This portion of the development cost will also be dependent upon the scenario chosen and could require as much as 20% additional effort (i.e., 1.5 person months) for the implementation of scenario 1. This additional level of effort would decrease (percentage wise) with other scenarios but overall could increase slightly. The total level of effort for each identified scenario is discussed in the following sections.

6.1 PRESTO and Additional Pathways

Table 6-1 presents an overview of the level of effort required for each scenario. For Scenario 1 (i.e., the installation of PRESTO upon AECB's HP1000 and addition of pathways (mechanisms) it can be seen that the total level of effort required is 7.25 person months. Of this total, 2.25 person months would be associated with installation (including conversion and segmentation), associated quality assurance functions and instruction to AECB personnel. This estimate is based on the level of effort required for conversion of PRESTO to an IBM-PC/AT (approximately 0.5 person months). It should be emphasized the IBM-PC/AT version used to obtain an estimate of turnaround does not satisfy AECB requirements.

The costs associated with the implementation of additional pathways/mechanisms is based on an evaluation of the complexity of the necessary software modification and reflects the fact that the gas pathway will be one of the most significant to incorporate due to the variety of potential ways of simulating this process for both normal operation and resident intruder (basement) scenario. The fish/game ingestion pathway would also require significant effort since the groundwater contribution to the surface water would be required. Water immersion dose would also require the addition of this capability but, for the purpose of this cost proposal, has been excluded from this task (to avoid duplication). The remaining task represents a combination of all remaining pathways mechanisms to be incorporated including wet deposition, sediment effects and shielding due to snow cover.

6.2 PRESTO, Additional Pathways and User Friendly Capability

Table 6-1 presents the level of effort required to incorporate user friendly pre- and post-processors to PRESTO in addition to the capability provided under Scenario 1. Based on INTERA's familiarity with the development of such items as menu-driven input routines and

Table 6-1 Level of Effort for PRESTO Implementation Scenarios (person months)

	QA	Code Development	Instruction Training	Total
Scenario 1				
Installation	0.75	1.0	0.5	2.25
Pathways/Mechanisms				
Radon Gas	0.5	1.0	-	1.50
Fish/Game Ingestion	0.25	1.0	-	1.25
Immersion	0.25	0.5	-	0.75
Others	0.50	1.0	-	1.5
Total	2.25	4.5	0.5	7.25
Scenario 2 (user friendly)				
Scenario 1 Features	2.25	4.5	0.5	7.25
Input Pre-processor	1.0	4.0	0.5	5.5
Output Post-processor	1.0	6.0	0.5	7.5
Total	4.25	14.5	1.5	20.25
Scenario 3 (probabilistic capability)				
Scenario 1 Features	2.25	4.5	0.5	7.25
Input Pre-processor	1.0	5.0	0.5	6.5
Mainframe Driver	3.0	8.0	-	11.0
Output Post-processor	1.0	7.0	0.5	8.5
Total	7.25	24.5	1.5	33.25
Scenario 4 (full capability)				
Scenario 1 Features	2.25	4.5	0.5	7.25
Additional Features	6.0	6.0	1.0	13.0
Input Pre-processor	1.0	5.0	0.5	6.5
Mainframe Driver	3.0	8.0	-	11.0
Output Post-processor	1.0	7.0	0.5	8.5
Total	13.25	30.5	2.5	46.25

post processors having statistics and graphics capability, it is anticipated that an additional 13 person months would be required to develop this software without the use of existing code.

6.3 PRESTO, Additional Pathways and Probabilistic Capability

The additional level of effort required to incorporate a probabilistic capability into PRESTO (specifically a sampling methodology) is reflected in the development of a mainframe driver program and the additional effort associated with pre- and post-processors. The mainframe driver would be responsible for performing the sampling, correlation of input variables, bookkeeping, determination of partial rank correlation coefficients, etc. The level of effort associated with this task reflects the fact that it is a major software development task. The increase in the level of effort associated with the pre- and post-processors reflects the additional requirements resulting from a sampling capability. This would include the generation of pdf's for the pre-processor and the additional data manipulation requirements created by the sampling methodology. The level of effort required for the development of the pre-, post-processors and mainframe driver would be approximately 6.5, 11.0 and 8.5 person months, respectively.

6.4 Full Capability Version

The additional capability provided under this scenario is reflected in the task labelled "Additional Features". This task would include modularity enhancement, incorporation of variable time step, pathway selection, run time diagnostics, explicit liner properties, addition of user specified variables for hard programmed values, and provision of a self teaching curriculum. The high level of QA associated with this task (6 person months) reflects the extent of the modifications. Approximately 13 person months would be required to fulfill this additional task.

6.5 Cost Reduction Alternatives

In recognition of the fact that the level of effort contained in the scenarios examined is high, INTERA is recommending that the following be considered as cost-cutting measures:

1. Use of existing software especially for pre- and post-processors. INTERA for example has developed significant software for graphics and user friendly interfaces. This software could be used at a cost far less than that of developing the software without the use of existing code.

2. Consider cost sharing within AECB. Much of the proposed software could be developed to be generic and multi-purpose in nature. This would especially apply to post-processors having graphical capability and statistical capability which could be used by other programs/facets of AECB.

3. Undertake the joint development of software with external agencies on a cost sharing basis.

7. CONCLUSIONS AND RECOMMENDATIONS

Although it might seem that PRESTO has significant deficiencies in terms of its ability to meet AECB requirements the following items should be considered:

- The requirements of AECB are extensive and reflect the needs/desires of a diverse group of potential users;

- Of all existing publically available models, PRESTO most closely fulfills the needs of AECB. The additional software modifications required to satisfy AECB requirements would still be significantly cheaper than development of their own model without the use of the existing code. As an example, UTAP development costs are now in excess of $800,000 (DSS, 1986).

The costs of upgrading PRESTO to completely satisfy all AECB requirements is high and only AECB can assess whether the final capability could justify the costs. However, the following items should be considered in evaluating the options available to AECB.

1. PRESTO would provide an independent analysis capability to evaluate licencee applications.

2. Costs could be reduced by using existing software and code.

3. New hardware will be required to provide a probabilistic capability.

In view of these facts, it is recommended that AECB consider at least Scenario 1 for implementation together with the user friendly input pre-processor from Scenario 2. This would provide AECB with all of the possible pathways for radionuclide migration, the additional mechanisms identified in this study and ensure that those individuals with limited computer literacy could easily create/edit data sets and perform simulations. Although outputs would have to be restricted to hard copy, little training is required to learn how to interpret these outputs. This combination of scenarios would provide AECB with a useable deterministic capability for slightly less than 13 person months. This cost could also be reduced through implementation of some of the cost saving alternatives identified in Section 6.5. At the very least, it is strongly recommended that the installation of PRESTO (the first task of Scenario 1) be undertaken to provide AECB with some form of independent capability.

REFERENCES

Anspaugh, L.R., J.J. Shinn, P.L. Phelps, and N.C. Kennedy, 1975. Resuspension and Redistribution of Plutonium in Soils. Health Phys. 29:571-582.

Atomic Energy Control Board, 1986. Proposed Amendments to the Atomic Energy Control Regulations. Consultative Document C-83.

Begovich, C.L., K.F. Eckerman, E.C. Schlatter, and S.Y. Ohr, 1981. DARTAB: A Program to Combine Airborne Radionuclide Environmental Exposure Data to Generate Tabulations of Predicted Impacts. ORNL-5692 (Oak Ridge National Laboratory, Oak Ridge, Tennessee).

Briggs, G.A., 1973. Diffusion Estimation for Small Emissions. ATDL Contribution File No. 79. National Oceanographic and Atmospheric Administration, Atmospheric Turbulence and Diffusion Laboratory.

Department of Supply and Services (DSS) Canada, 1986. Research and Development Bulletin No. 165.

Dunning, D.E., Jr., R.W. Leggett, and M.G. Yalcintas, 1980. A Combined Methodology for Estimating Dose Rates and Health Effects from Exposures to Radioactive Pollutants. ORNL/TM-7105 (Oak Ridge National Laboratory, Oak Ridge, Tennessee).

Fick, A., 1855. VEBER Diffusion. Jour. Ann. Phys. Leiptzig, Vol. 170, p. 59-86.

Fields, D.E. and C.J. Emerson, 1984. Unrestricted Disposal of Minimal Activity Levels of Radioactive Wastes: Exposure and Risk Calculations. ORNL-6001.

Fields, D.E. and C.W. Miller, 1980. User's Manual for DWNWND--An Interactive Gaussian Plume Atmospheric Transport Model with Eight Dispersion Parameter Options. ORNL/TM-6874 (Oak Ridge National Laboratory, Oak Ridge, Tennessee).

Freeman, H.D. and J.N. Hartley, 1984. Predicting Radon Flux from Uranium Mill Tailings. Sixth Symposium on Uranium Till Tailings Management, Fort Collins, Colorado.

GTC Geologic Testing Consultants Ltd., 1985. Shallow Disposal of Radioactive Waste Survey of Models. AECB Report INFO-0149.

Hillel, D. and C. van Bavel, 1976. Simulation of Profile Water Storage as Related to Soil Hydraulic Properties. J. Soil Science Soc. of Am., Vol. 40, No. 6, November.

Hung, C.Y., 1983. A Model to Simulate Infiltration of Rainwater Through the Cover of a Radioactive Trench under Saturated and Unsaturated Conditions. In Role of the Unsaturated Zone in Radioactive and Hazardous Waste Disposal, edited by J.W. Mercer et al., Ann Arbor Science, 1983.

Hung, C.Y., 1981. An optimum model to predict radionuclide transport in an aquifer for the application to health effects evaluation. In Proceedings, Modeling and Low-Level Waste Management: An Interagency Workshop held December 1-4, 1980, Denver, Colorado, (C.A. Little and L.E. Stratton, compilers), pp. 65-80, ORO-821 (Department of Energy, Oak Ridge Operations Office, Oak Ridge Tennessee).

Little, C.A., D.E. Fields, C.J. Emerson, G. Hiromoto, 1981. Environmental Assessment Model for Shallow Land Disposal of Low-Level Radioactive Wastes: Interim Report. ORNL/TM-7943 (Oak Ridge National Laboratory, Oak Ridge, Tennessee).

Mayer, D.W., C.A. Oster, R.W. Nelson, G.W. Gee, 1981. Radon Diffusion Through Multilayer Earth Covers. Pacific Northwest Laboratory Report PNL-3989.

McMahon, T.A., and P.J. Denison, 1979. Empirical Atmospheric Deposition Parameters - A Survey. Atmospheric Environment 13:571-85.

Moore, R.E., C.F. Baes III, L.M. McDowell-Boyer, A.P. Watson, F.O. Hoffman, J.C. Pleasant, and C.W. Miller, 1979. AIRDOS-EPA: A Computerized Methodology for Estimating Environmental Concentrations and Dose to Man from Airborne Releases of Radionuclides. ORNL-5532 (Oak Ridge National Laboratory, Oak Ridge, Tennessee).

Pasquill, F., 1976. The "Gaussian Plume" Model with Limited Vertical Mixing. U.S. Environmental Protection Agency, Research Triangle Park, N.C. Report EPA-600/4-76-042.

Pasquill, F., 1961. The estimation of the dispersion of windborne material. Meteorol. Mag. 90:33.

Philip, J.R., 1974. Water Movement in Soil. Ed. D.A. DeVaries and N.H. Afgan, Halsted Press-Wiley, New York.

Ripple, C.C., J. Rubin and T. Van Hylkama, 1972. Estimating Steady-State Evaporation Rate from Bare Soil under Conditions of High Water Table. U.S. Geological Survey, Water Supply, pp. 2019-A.

Rogers, V.C., K.K. Nielson and G.N. Gnugnoli, 1980. Calculation of Radon Fluxes from Covered Uranium Piles. Symposium on Uranium Mill Tailings Management, Fort Collins, Co.

Van Zettan, J.A., 1986. Personal communication.

Wischmeier, W.H. and D.D. Smith, 1965. Predicting Rainfall-Erosion Losses on Cropland East of the Rocky Mountains. Agricultural Handbook 282 (USDA, Ag. Research Serv.).

APPENDIX A

Input Variables
PRESTO-CPG*

*from "PRESTO-CPG: User's guide and documentation for critical population group modifications to the PRESTO code", prepared for U.S. Environmental Protection Agency, by Rogers and Associates Engineering Corporation, October, 1984

4. USER INPUT TO PRESTO-CPG

There are basically three types of data that are needed to execute PRESTO-CPG. They are: (1) site-specific and radionuclide data used in the transport section of the code for calculating concentrations, (2) data used specifically by DARTAB submitted for creating tabular output, and (3) dosimetric and health effects data used by the DARTAB submodel. The latter is a magnetic tape file previously created by the RADRISK program and as such requires no user action or data other than identification of the appropriate file in the job JCL.

In PRESTO-CPG the site/transport data are entered in two data sets. The first set contains all physical and chemical site transport and radionuclide parameters except that data required for the trench infiltration calculations. These data constitute the second site/transport input data set. The deep disposal options of PRESTO-CPG do not require the infiltration calculation, and as a result the second site/transport data set are not required or read in. When the shallow disposal option of PRESTO-CPG is utilized, the infiltration data set is still required, however.

The first of the two site/transport data sets and the DARTAB-specific data set are concatenated, existing as a single input file. When used, the infiltration data set is a second file. The dosimetric and health effects data created by RADRISK constitutes the third file required by PRESTO-CPG. These three files are read on logical units 5, 4 and 25, respectively. The data set/file relations are shown in Figure 4-1. For the remainder of this chapter attention is focused on the specific input requirements of the PRESTO-CPG program.

4.1 SITE/TRANSPORT DATA

The site/transport data set consists of both character and numeric data. The data is read in SUBROUTINE SOURCE and is formatted. The descriptions of the card sequence for this data set follow.

CARD 1 TITLE (20A4).
TITLE - Identifies the run - 80 characters allowed.

CARD 2 LOCATE (20A4).
LOCATE - Lists the location of the site - 48 characters allowed.

CARD 3 MAXYR, NONCLD, LEAOPT, NYR1, NYR2, IOPVWV, IOPSAT, IPRT1, IPRT2, IDELT, IRRES1, IRRES2, LIND, IAVG1, IAVG2, IDISP (16I5).

MAXYR - The number of years for which the simulation will run.

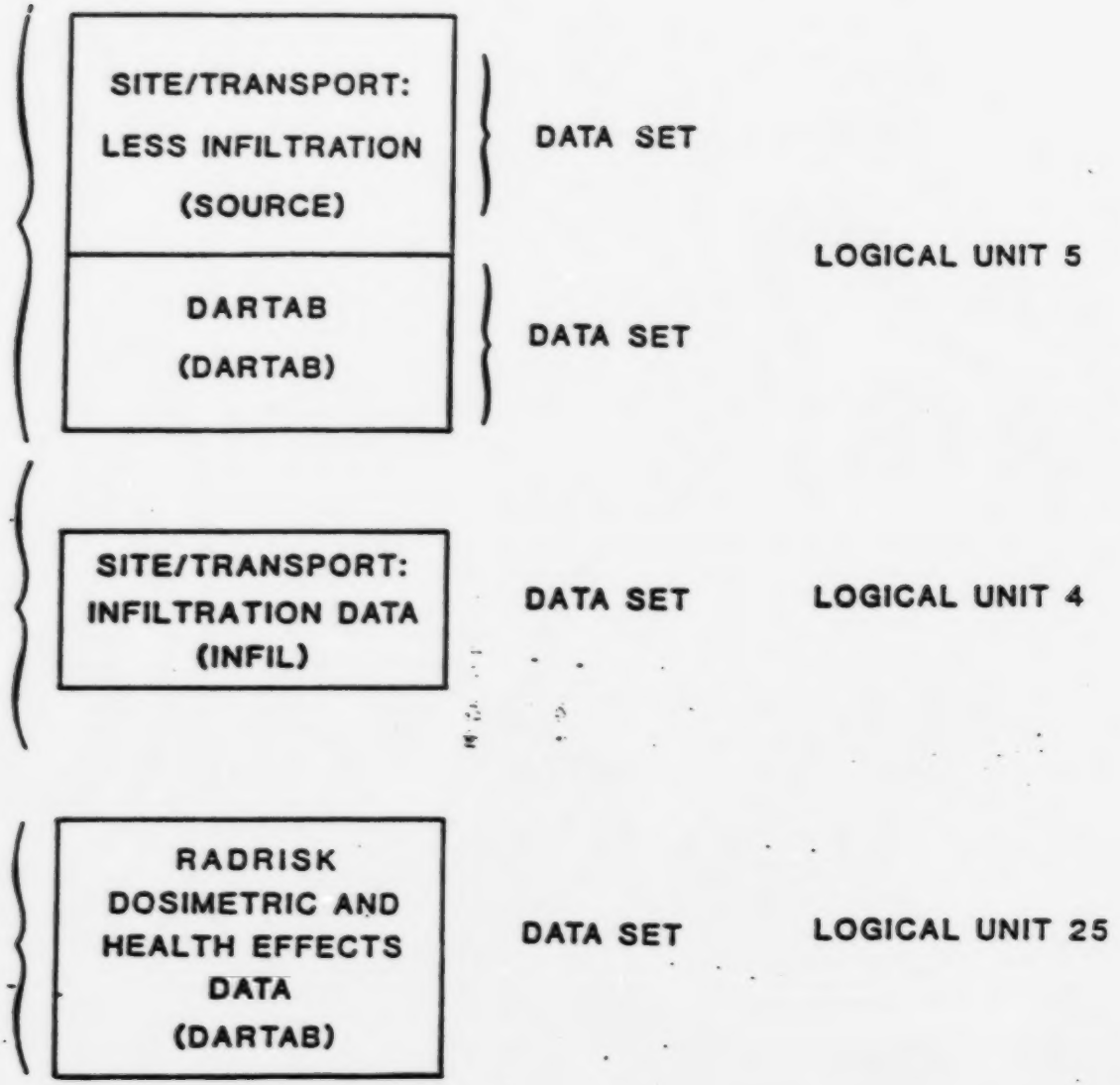


FIGURE 4-1. PRESTO-DEEP INPUT FILES.

NONCLD - The number of radionuclides which are used in the simulation; must be 40 or less.

LEAOPT - The leaching option. Radionuclides will be removed from trench in different manners depending on the value of LEAOPT - Must be 1-5 according to the following calculation methods:

Option	Leach Calculation Method
1	Total contact, distribution coefficient
2	Immersed fraction, distribution coefficient
3	Total contact, solubility
4	Immersed fraction, solubility
5	Release fraction

NYR1, NYR2 - Beginning and ending years of cap failure function Both values must be less than or equal to MAXYR. NYR2 must be greater than or equal to NYR1.

IOPVWV - Option for farming directly into the waste.

- = -1 no farming into the waste
- = 0 farming into the waste

IOPSAT - No longer in use.

IPRT1, IPRT2, IDELT - Variables to control beginning year of annual summary, ending year, and the time step between printing, respectively. An annual summary will be printed for each year between years IPRT1 and IPRT2 into which IDELT divides evenly.

IRRES1, IRRES2 - Beginning and ending year of mechanical suspension of contaminated soil into atmosphere. Used for farming scenario.

LIND - Option parameter passed to DARTAB to calculate health effects. If LIND = 0, then DARTAB computes concentrations and rates for maximally exposed individuals. If LIND = 1, then general population concentrations are computed.

IAVG1, IAVG2 - Beginning and ending years for averaging nuclide concentration values.

IDISP - Mode of disposal. IDISP = 1, 2, 3, or 4 for shallow land burial, deep well injection, hydrofracture, and deep geologic disposal, respectively.

CARD 4 IVAP, IBSMT, IAQSTF, IRST ITWO (5I5).

IVAP - Not used.

IBSMT - The beginning year for the basement correction factor for surface gamma exposure calculations made by DARTAB. If IBSMT = 0, correction factor is calculated beginning in that year. If IBSMT = -1, then no correction is calculated.

IAQSTF - Control parameter for aquifer to stream flow. A blank field defaults to calculations under the assumption that the flow takes place, otherwise the field should contain a nonzero integer.

IRST - Number of years for restricted site use after site closure.

ITWO - Secondary year for which an organ dose summary table will be output.

CARD 5 PCT1, PCT2, WWATL, WWATA, WWATH, SWATL, SWATA, SWATH (8F10.0).

PCT1, PCT2 - The fraction of the cap that is assumed to fail by some artificial means in years NYR1 and NYR2, respectively.

Failure of the cap constitutes total removal of all cap, of OVER Thickness, for PCT1 of the trench area in NYR1 and for PCT2 of the trench area in NYR2. Between NYR1 and NYR2 a linear interpolation between pairs (NYR1, PCT1 and NYR2) calculates the amount of the trench area that is totally bare. Even if PCT1 and PCT2 are set at zero, the trench cap may ultimately fail through erosion; see function CAP and subroutine ERORF.
WWATL - Fraction of well water used for irrigation (1.0 if water comes from well, 0.0 if none).

WWATA - Fraction of well water used for animals (1.0 if water comes from well, 0.0 if none).

WWATH - Fraction of well water used by humans (1.0 if water comes from well, 0.0 if none).

SWATL - Fraction of surface water used for irrigation (1.0 if all water comes from surface, 0.0 if none).

SWATA - Fraction of surface water used for animals (1.0 if all water comes from surface, 0.0 if none).

SWATH - Fraction of surface water used by humans (1.0 if all water used comes from surface, 0.0 if none).

CARDS 6-12 Comments (20A4).

These cards available for comments and reference pertaining to data set.

CARD 13 TAREA, TDEPTH, OVER, PORT, DENCON, RELFAC, CPRJ, SINFL (8F10.0).

TAREA - The total combined facility surface area for the hypothetical facility being simulated (m^2). Must be nonzero.

TDEPTH - Nominal depth (m) of operating trench in the shallow disposal scenario. Waste thickness in deep scenarios.

OVER - Thickness of trench overburden (m).

PORT - Porosity of material within trench. Must be nonzero.

DENCON - Mean density of the waste materials in the trench (g/cm^3).

RELFAC - The annual fraction of the total trench inventory of each radionuclide that is released if LEAOPT is chosen 5 (see Card 3).

CPRJ - Complement to fraction of underground water flowing to the stream.

SINFL - Annual infiltration rate for noncap portions of the site and for local farmland (m/yr).

CARD 14 SSAT, RESAT (2F10.0).

SSAT - Fraction of saturation for formation beneath the buried waste. If 0, the fraction of saturation is calculated internally by the code.

RESAT - Fraction of residual saturations.

CARD 15 PERMT, FACTIM, TMN, CFT1, DCFT, FGAM (6F10.0).

PERMT - Trench permeability (m/yr).

FACTIM - Number of years of active operation of the site.

TMN - Number of years of active maintenance after site closure. No nuclide migration is initiated during the maintenance period.

CFT1 - Number of years before waste containers begin failing.

DCFT - Number of years after CFT1 that containers fail. At time CFT1+DCFT all containers have failed.

FGAM - Dimensionless factor characterizing the intensity and duration of gamma exposure from the basement scenario.

CARD 16 DTRAQ, DWELL, GWV, AQTHK, AQDISP, PORA, PORV, PERMV (8F10.0).

DTRAQ - The distance from the bottom of the trench to the nominal depth of the aquifer (m). DTRAQ + TDEPTH + OVER should equal the aquifer depth below surface.

DWELL - Distance from the trench to the well used for irrigation and drinking (m). Must be entered, nonzero.

GWV - Velocity of the groundwater in the aquifer (m/yr). Must be entered, nonzero.

AQTHK - Thickness of the aquifer at the location of the well (m). This is used to calculate the volume of water in which the available radionuclides are diluted. Must be entered, nonzero.

AQDISP - Dispersion angle of the pollutant plume in the aquifer (radians). Used with AQTHK to calculate dilution volume. Must be entered in radians.

PORA - Aquifer porosity.

PORV - Sub-trench porosity.

PERMV - Sub-trench permeability (m/yr).

CARD 17 VWV, HGRAD, FRACB, ALV, ALH, BDENV (6F10.0).

VWV - Vertical water velocity (m/yr). If a value of 0.0 is input, VWV is calculated internally.

HGRAD - Hydraulic gradient (dimensionless). If a value of 0.0 is input, HGRAD is assigned the default value 1.0.

FRACB - Fraction of waste impacted ($0. < FRACB \leq 1.0$). The default value is 1.0.

ALV - Dispersivity in the confining stratum (m), i.e., the region beneath the trench (IDISP = 1) or the aquiclude (IDISP = 2, 3, or 4). The default value is 0.3 m.

ALH - Dispersivity in the aquifer (m). The default value is 0.3 m.

BDENV - Density of the confining stratum (g/cm^3).

CARD 18 H, VG, U, VD, XG, HLID, ROUGH (7F10.0).

H - Atmospheric source height (m). One meter, chosen because most resuspension rate measurements are expressed for that height.

VG - Fall velocity of contaminated soil particles due to gravity (m/s).

U - Annual average wind speed (m/s) in the direction of interest. For population calculations, the wind speed toward the population centroid. Must be entered, nonzero.

VD - Deposition velocity (m/s). Nominal generic value is 0.01 m/s.

XG - Distance from source (trench) to population or individual of interest (m).

HLID - Height of the inversion layer or lid (m).

ROUGH - Hosker's roughness parameter (m).

CARD 19 FTWIND, CHIQ, RE1, RE2, RE3, RR, FTMECH (7F10.0).

FTWIND - Fraction of the time wind blows toward the population or individual of interest.

CHIQ - The user-specified dispersion coefficient for the population of interest may be calculated by an external atmospheric dispersion code. A nonzero value will override any calculation of atmospheric dispersion within code.

RE1, RE2, RE3 - Factors (including algebraic signs) in the resuspension rate equation.

RR - During the period between years IRRES1 and IRRES2, the resuspension rate RR (sec^{-1}) will be included as a source term to subroutine AIRTRM. For on site reclaimer, RR is the dust loading of the inhaled air (gm/m^3).

FTMECH - The rate of resuspension, RR, will be modified by this fraction, which has a value between zero and unity.

CARD 20 IT, IS (2I5).

IT - Indicator variable for type of stability class formulation. Suggested formulation is Pasquill-Gifford, IT = 1.

IS - Stability category indicator. Values of 1-6 correspond to stability categories of A-F. Single value represents most common stability category from nearest meteorology station to site of interest.

CARD 21 RAINF, ERODF, STPLNG, COVER, CONTRL, SEDELR (6F10.0).

RAINF - The rainfall factor.

ERODF - The soil-erodibility factor has units of tons/acre-R, where R = RAINF above.

STPLNG - The slope steepness-length factor.

COVER - The crop management factor.

CONTRL - The erosion control practices factor.

SEDELR - The sediment delivery ratio. This ratio is intended to apply to fouling of waterways from construction activity.

CARD 22 PORS, BDENS, STFLOW, EXTENT, ADEPTH (5F10.0).

PORS - Porosity of the surface soil. Must be nonzero.

BDENS - Bulk density of the soil (g/cm^3). Must be entered nonzero.

STFLOW - Annual flow rate of the nearest stream (m^3/y). Must be nonzero.

EXTENT - The cross slope extent of the surface region contaminated by operational spillage (m). Must be nonzero.

ADEPTH - The active depth of soil in the surface-contaminated region (m). Used for calculation of radionuclide concentration in both surface soil and surface water. Must be nonzero.

CARD 23 PD, PPN, RUNOFF, SEEP (4F10.0).

PD - Distance from trench to nearest stream (m). Must be nonzero.

PPN - Total annual precipitation (m).

RUNOFF - Fraction of the annual precipitation that runs off annually.

SEEP - The fraction of the total annual precipitation (PPN) that ultimately becomes deep infiltration. This variable is zero unless one is conducting <u>parametric</u> studies for the shallow land burial option.

CARD 24 Y1, Y2, PP, XAMBWE, TA, TE1, TE2 (7F10.0).

Y1, Y2 - Agricultural productivity for pasture grass and other consumed vegetation respectively (kg/m^2).

PP - Surface density of soil (kg/m^2). Assumes a 15 cm plow depth. For farming scenario, this value should be in agreement with the value of BDENS, CARD 20. Must be nonezero.

XAMBWE - The weathering removal decay constant for atmospheric deposition onto foodcrops (h^{-1}).

TA - Not used.

TE1, TE2 - Period of time that pasture grass or crops/leafy vegetables, respectively, are exposed to contaminated air during each growing season (h).

CARD 25 TH1, TH2, TH3, TH4, TH5, TH6, FP, FS (8F10.0).

TH1-TH6 - These six variables represent the delay time between harvest and consumption by animal or man of pasture grass, stored feed, leafy vegetables for maximum individual, produce for maximum individual, and leafy vegetables and produce for the general population, respectively.

FP - Fraction of each year the animals graze on pasture grass.

FS - This variable is the fraction of an animal's daily feed that is fresh grass for the period of time animals are in pasture.

CARD 26 QFC, QFG, TF1, TF2, TS, ABSH, P14 (7F10.0).

QFC - The amount of feed consumed daily by cattle (kg).

QFG - The amount of feed consumed daily by dairy goats (kg).

TF1, TF2 - The transport time (h) from animal feed into milk and into the receptor human for the maximum individual and the general population exposures, respectively.

TS - Length of time between slaughter of animal and human consumption of the resultant meat (h).

ABSH - The absolute humidity of the atmosphere (g/m^3). Used in specific activity foodchain calculations for tritium concentrations in foodstuffs. Must be nonzero.

P14 - The fractional equilibrium ratio for C-14.

CARD 27 XRTM, RTGR (2F10.0).

XRTM - Maximum root depth for on-site farming scenario (m).

RTGR - Root growth rate constant (yr^{-1}).

CARD 28 TW, FI, WIRATE, QCW, QGW, Q8W, (6F10.0).

TW - Not used.

FI - Fraction of the year that crops are irrigated.

WIRATE - Irrigation rate (l/m^2-h). Application time is set equivalent to number of frost-free days for county.

QCW, QGW, Q8W - Values for the amount of water (l/d) consumed by milk cows, milk goats, and beef cattle, respectively.

CARD 29 ULEAFY, UPROD, UCMILK, UGMILK, UMEAT, UWAT, UAIR, POP (8F10.0).

ULEAFY - The human uptake of leafy vegetation (kg/yr).

UPROD - The human uptake of produce (kg/yr).

UCMILK - The human uptake of cow milk (l/yr).

UGMILK - The human uptake of goat milk (l/yr).

UMEAT - The human uptake of meat (kg/yr).

UWAT - The human uptake of drinking water (l/yr).

UAIR - The inhalation rate (m^3/yr).

POP - Population.

CARD 30 RELFRC(1), RELFRC(2), RELFRC(3), RELFRC(4), RELFRC(5), FTRAB, FRTRSH (7F10.0).

RELFRC(1) - The release fraction for the absorbing waste. This array elements is currently not used and is set equal to 0.0.

RELFRC(2) - The release fraction for the activated metals.

RELFRC(3) - The release fraction for the trash.

RELFRC(4) - The release fraction for the solidified waste.

RELFRC(5) - The release fraction for the incinerated/solidified waste.

FTRAB - The fraction of trash that is absorbing material.

FRTRSH - The fraction of waste that is not in water-tight containers.

CARD 31 SPLAW, SPLAM, SPLTR, SPLSW, SPLIS (5F10.0).

SPLAW - Spillage fraction for absorbing waste.

SPLAM - Spillage fraction for activated metal waste.

SPLTR - Spillage fraction for trash.

SPLSW - Spillage fraction for solidified waste.

SPLIS - Spillage fraction for incinerated solidified waste.

CARD SET 32 This card is repeated for each nuclide, I.

CARD 32 NUCLIDE(I), (NUCL(I,K),K=1,8), CIAW(I), CIAM(I), CITR(I), CISW(I), CIIS(I) (A8, T1, 8A1, 2X, 5F10.0).

NUCLID(I) - The name of the radionuclide as used in the code. Must be written left justified and with no imbedded blanks and a hyphen separating the alphameric and numeric. The names used must agree with the conventions used in RADRISK and DARTAB.

NUCL(I,K) - Not used.

CIAW(I) - Amount of the radionuclide in the absorbing waste (Ci).

CIAM(I) - Amount of the radionuclide in the activated metals (Ci).

CITR(I) - Amount of the radionuclide in the trash (Ci).

CISW(I) - Amount of the radionuclide in the solidified waste (Ci).

CIIS(I) - Amount of the radionuclide in the incinerated/ solidified waste (Ci).

CARD SET 33, 34, 35+ This grouping of three cards is repeated for each nuclide, I.

CARD 33 NUCLID(I), (NUCL(I,K),K=1,8), DUMMY, SOAM(I), STAM(I), ATAM(I), DECAY(I), SOL(I), CON(I), (A8, T1, 8A1, 2X, F10.0).

NUCLID(I) - The name of the radionuclide as used in the code. Must be written left justified and with no imbedded blanks and with a hyphen separating the alphameric and numeric. The names used must agree with the conventions used in RADRISK and DARTAB.

NUCL(I,K) - Not used.

DUMMY - Not used.

SOAM(I) - Not used.

STAM(I) - The amount of radioactivity placed into the stream nearest the site at the beginning of the simulation (Ci).

ATAM(I) - The concentration of radioactivity of each radionuclide (Ci/m^3) placed into the air directly above the trench at the beginning of the simulation.

DECAY(I) - The radiological decay constant (y^{-1}). As input is equal to ln 2 divided by the radiological halflife.

SOL(I) - The solubility of the radionuclide stored in the trench (g/ml). SOL is used only if LEAOPT = 5.

CON(I) - Conversion factor for global health effects (health effects/Ci released).

CARD 34 NU, XKD(1,I), XKD(2,I), XKD(3,I), XKD(4,I) (A8, 2X, 4F10.0).

NU - Radionuclide name (same as on Card 32).

XKD(1,I) - Surface K_d of radionuclide I (ml/g).

XKD(2,I) - Waste K_d of radionuclide I (ml/g).

XKD(3,I) - Vertical zone K_d of radionuclide I (ml/g).

XKD(4,I) - Aquifer K_d of radionuclide I (ml/g).

CARD 35 NC, RA(I), RW(I), BV(I), BR(I), FMC(I), FMG(I), FF(I) (A8, 2X, 7F10.0).

NC - Radionuclide name (same as Card 32).

RA(I) - Radionuclide retention fraction for air.

RW(I) - Radionuclide retention fraction for irrigation.

BV(I) - Radionuclide soil-to-plant uptake factor for vegetative parts.

BR(I) - Radionuclide soil-to-plant uptake factor for grain.

FMC(I) - Radionuclide forage-to-milk transfer factor for cows.

FMG(I) - Radionuclide forage-to-goat transfer factor for goats.

FF(I) - Radionuclide forage-to-beef transfer factor.

4.2 DARTAB DATA

The DARTAB user input provides the user options for processing the exposure data, dosimetric data, and of tabulations of output. The first data card is a title card. The remaining data are read using IBM FORTRAN NAMELIST format. The order of data items in a NAMELIST group is not important, but arrays that refer to nuclides should have the constants in the same order as occurred in the site/transport data. The end of a NAMELIST group is designated by &END. An example of this input can be seen in the sample problem. The NAMELISTS are read from logical unit number 5 and must follow directly after the site/transport data. The input utilized by DARTAB are as follows.

Title Card
(20A4)

Namelist INPUT:

ILOC, JLOC are the direction indices of the exposure array that is used to locate an individual for which a dose or risk table is printed. AIRDOS-EPA, the code for which DARTAB was orignally written, supplied a two-dimensional exposure array to DARTAB. The PRESTO codes, however, supply only a mean exposure value for each of air concentration, ground surface concentration, collective inhalation rate and collective ingestion rate, for only one location. These values are the first entry of the array; hence, both indices should be specified as 1.

PLOC is an indirect indicator of location. Because PRESTO-MID does not provide a two-dimensional exposure array to DARTAB, PLOC should be set to 100 or omitted.

AGEX is the current mean life expectancy.

ILET. For LLW disposal site simulations with a mixture of nuclides, ILET should be set to 1.1 meaning a combined LET table for both dose and risk tables. For the intrusion scenario, where external exposures are of greater importance, the user may with to set ILET to 2.2.

DTABLE, RTABLE, FTABLE. These variables, each dimensioned by seven, indicate which type of detailed dose, risk and risk equivalent table, respectively, will be printed. The type of table printed for each position in the variable array is shown below. A zero entered for a given array position indicates that no table of that type will be printed. A value of one will lead to a table for the "selected individual." This is the value which should be used in PRESTO-MID.

OUTPUT is the nuclide dose factor output status flag. If specified, TRUE, then NONCLD pages, one per radionuclide, will be output to list the dose rate factors.

GSCFAC is the groundsurface correction factor.

Namelist ORGAN: NORGN is an integer and is the number of organs considered in dose determination.

ORGN is the array of double precision names for these organs. There are NORGN entries.

TIME is the time associated with the dose commitment (yr). There are NORGN entries.

Array Position	Table Type	Column	Row	Table Label
1	a	Organs or cancers	Radionuclides	Individual pathways
2	b	Organs or cancers	Radionuclides	External and internal
3	c	Organs or cancers	Radionuclides	All pathways
4	d	Radionuclides	Pathways	Organs or cancers
5	e	Organs or cancers	Pathways	Radionuclides
6	f	Radionuclides	Pathways	Summed over organs or cancers
7	g	Organs or cancers	Pathways	Summed over nuclides

Namelist QFACTOR:

HLET is the relative biological effectiveness factor to be used in the case of high-LET dose rates for conversion of absorbed dose to dose equivalent. There are NORGN entries.

LLET is the relative biological effectiveness factor to be used in the case of low-LET dose rates for conversion of absorbed dose to dose equivalent. There are NORGN entries.

Namelist CANCER:

NCANC is the number of cancers considered. CANC is an array containing the double precision names of the cancers under consideration. There are NCANC entries.

RELABS is a flag denoting use of either an absolute risk (=1) or relative risk (=2) model.

Namelist GENTIC:

GENEFF is a logical variable indicating the output status of genetic effects. If GENEFF = .TRUE. the genetic effects are output. If GENEFF = .FALSE. the genetic effects are not output.

NGEN is the number of organs considered for genetic effects.

GEN is the array of double precision names of those organs considered for genetic effects. There are NGEN entries.

GRFAC(1) and GRFAC(2) are the risk conversion factors corresponding to low-LET and high-LET doses, respectively (genetic effects per rad/million births).

REPPER is the population replacement rate.

GLLET is the relative biological effectiveness factor for converting low-LET genetic doses to dose equivalents. There are NGEN entries.

GHLET is the relative biological effectiveness factor for converting high-LET genetic doses to dose equivalents. There are NGEN entries.

Namelist RNUCLD:

NONCLD is the number of radionuclides and must be equivalent to the same variable in transport portion of code, Code 3, but always less than or equal to 40.

NUCLID is the array of alphanumeric names of the NONCLD radionuclides. The order of the names must be the same order as in transport section of input cards 29+.

PSIZE is the median aerodynamic diameter associated with each radionuclide (microns). There are NONCLD entries.

RESP denotes the respiratory clearance class, either day ('D'), week ('W'), year ('Y'), gas ('*'), or not used (' '). There are NONCLD entries.

GLABS is the absorption factor for each of the four segments of the GI tract for each nuclide (must be entered). The DARTAB code expects to read a value for each segment (stomach, small intestine, upper large intestine, and lower large intestine). There are four entries for each nuclide.

Namelist LOCTAB:

NTLOC is the number of location tables to be output.

RNLOC is the radionuclide to use for the table. SUM results in the sum of all nuclides, WORKLEVL results in working level calculations, WLSUM results in total risk for all nuclides.

OGLOC is the organ or cancer to use for the table. SUM results in the sum of all cancers.

PTLOC specifies the pathway to use in printing the location table. Values of 1-7 will result in ingestion, inhalation, air immersion, ground surface exposures, internal exposures (sum of ingestion and inhalation), external exposures (sum of air immersion and ground surface exposures), and total, respectively.

FALOC is the factor to be printed.

- 0 both high- and low-LET.
- 1 only combined LET table.
- 2 all three tables.

HELOC is the factor to be printed.

- 0 both high- and low-LET.
- 1 only combined LET table.
- 2 all three tables.

LTABLE indicates selected individual (LTABLE = 1), mean individual (LTABLE = 2), or collective group (LTABLE = 3). For PRESTO-MID LTABLE should be set equal to 1.

Namelist ORGANF:

NORGB is the number of organ dose weights to use to combine dose rates.

ORGDAT is the array of organ dose weighting factors. There are NORGB entries.

IPATH denotes the exposure pathway affected (1 = ingestion; 2 = inhalation; 3 = air immersion; 4 = ground surface; 5 = all pathways). There are NORGB entries.

ORGB are the organs to be used.

4.3 INFILTRATION DATA

The input data to the infiltration subroutine (INFIL) are read from input unit 4. Data for INFIL are of four types: Hydrologic and trench description characteristics; maximum day length in hours by month; daily mean temperatures by month; and hourly precipitation for nonzero precipitation events. The last card in the data set must have "99" in the first two columns. This data is only required when the shallow burial disposal option is used (IDISP = 1).

CARD 1 TWT, SLOP, XKI, EPSG, EPSP, YGMAX, XDE, XKE, YPI, YGI, (10F7.3).

TWT - Trench width (m).

SLOP - Trench cap slope.

XKI - Permeability of trench cover (m/hr).

EGSG - Porosity in gravity zone.

EPSP - Porosity in pellicular zone.

YGMAX - Trench cap thickness (m).

XDE - Equivalent upward diffusivity (m/hr).

XKE - Equivalent upward hydraulic conductivity (m/hr).

YPI - Pellicular infiltration capacity (m/hr).

TGI - Gravity infiltration capacity (m/hr).

CARD 2 DTH(1), DTH(2), ..., DTH(12) (12F5.1).

DTH(I) - Maximum day length for month I (January - December). There are 12 entries.

CARDS 3-33 TMP(1), TMP(2), ..., TMP(3) (2X,12F6.2).

TMP(I) - Daily mean temperature for month I (day C). There is one card for each day of the month, i.e., 31 cards.

CARDS 34+ MO, IDA, P(MO,IDA) (I2,1X,I2,1X,24F3.0).

MO - Month number.

IDA - Day of month (MO).

P(MO,IDA) - Hourly precipitation (units of 0.1 mm/hr).

CARD "last"

IAMP (I2).

IAMP - Must equal 99.

APPENDIX B

ICRP Dose
Calculation of Methodology

ICRP APPROACH TO DOSE CALCULATIONS

The AECB approach to the calculation is based on that recommended by the International Commission on Radiological Protection (ICRP) publications 26 and 30. In this approach, the dose equivalent is defined as:

$$H = DQN \qquad (B-1)$$

where: H = dose equivalent (sievert);
D = absorbed dose (gray);
Q = quality factor;
N = product of all other modifying factors (currently set to 1 by ICRP).

For radiation protection purposes, the ICRP has recommended the following values of Q for use with both internal and external radiation (ICRP, 1977):

Radiation	Q
X rays, γ rays, and electrons (beta particles)	1
Neutrons, protons, and singly charged particles of rest mass greater than one atomic mass unit	10
Alpha particles and multiply charged particles	20

The ICRP presents dose factors to calculate the dose equivalent to an exposed individual. The dose factor (or dose conversion factor) approach relates the organ dose equivalent to a unit amount of a radionuclide taken into the body by inhalation or ingestion. Knowing the actual intake rate of the radionuclide enables the actual organ dose to be calculated. Dose factors have also been calculated for sources external to the body.

ICRP (1977) has recommended an approach for combining doses so that the stochastic risk is the same regardless of whether the whole body is irradiated uniformly or there is non-uniform irradiation. This would include exposures to various organs from internally deposited nuclides as well as a combination of internal and external exposures. The approach uses the concept of an effective dose equivalent defined as:

$$H_E = \sum_j W_j H_j \qquad \text{(B-2)}$$

where: H_E = the effective dose eqivalent;

W_j = the weighting factor giving the proportion of the stochastic risk from the irradiation of organ j under uniform whole-body irradiation; and

H_j = the committed dose equivalent to organ j resulting from the intake of a unit amount of the radionuclide under consideration.

The values of the weighting factor W_j for several organs, as recommended by the ICRP, are shown below (ICRP, 1979):

Tissue or Organ	W_j
Gonads	0.25
Breast	0.15
Red bone marrow	0.12
Lung	0.12
Thyroid	0.03
Bone surfaces	0.03
Remainder	0.30

The quantity "collective dose equivalent" is used as a measure of the potential detriment to an exposed group of people and is defined by the ICRP as:

$$S = \sum_i H_i P_i \qquad (B\text{-}3)$$

where: S = the collective dose equivalent (also called "population dose");

H_i = the dose equivalent to the whole body or any specified organ or tissue to an individual in the exposed group;

P_i = the number of people receiving the dose equivalent of magnitude H_i.

The i index is used to denote the summing of the products H_i P_i over discrete dose intervals.

Differences between ICRP and PRESTO Approaches

The major differences between the ICRP and PRESTO approaches to dose calculation are:

- Differences exist in the units. ICRP units are newer Si units e.g., sieverts, becquerel, gray, etc. whereas PRESTO uses the older (conventionial) units rems, pico-curies, rad;

- Dose conversion factors used in PRESTO convert exposure to an absorbed dose whereas dose conversion factors supplied by ICRP convert an exposure to an equivalent dose.

Because these values and the quality factors are user supplied, changing from absorbed dose to equivalent dose is trivial. The values previously output as absorbed dose would then correspond to dose equivalents.

- PRESTO does calculate a value which is similar to the effective dose equivalent identified above (equation B-2) using Equation 2.27. The latter equation uses an absorbed dose instead of the dose equivalent used by the ICRP. Organ weighting factors are user supplied, so the use of ICRP factors is not a difficulty. If the ICRP dose conversion factors are used, these approaches would be identical.

- Although EPA claims that PRESTO calculates a population dose, it must be stressed that this approach assumes that all of the population resides at a single location. This is comparable to assuming that i = 1 in equation B-3. If there exist multiple population centres, PRESTO would have to be run multiple times to calculate a collective dose consistent with the approach outlined in equation B-3.

References

ICRP, 1977. International Commission on Radiological Protection. Radiation Protection. ICRP Publication 26. Pergamon Press.

ICRP, 1979. International Commission on Radiological Protection. Limits for Intakes of Radionuclides by Workers, Parts 1 and 2. ICRP Publication 30. Pergamon Press. Part 1, 1979; Part 2, 1980.

APPENDIX C

EPA Descriptions of PRESTO Routines*

*from "PRESTO-CPG: User's guide and documentation for critical population group modifications to the PRESTO code", prepared for U.S. Environmental Protection Agency, by Rogers and Associates Engineering Corporation, October, 1984

3.0 CODE DESCRIPTION

3.1 Subroutine Structure and Information Flow

The PRESTO-EPA-POP code is written in the FORTRAN IV language for an IBM 3081 or comparable computer system and requires 850K bytes of memory. It is designed to process up to 40 nuclides for a maximum of 10,000 years. Evaluation of local and basin health impacts of 31 radionuclides over 10,000 years takes approximately 7 minutes to execute. A shorter test of ten nuclides takes less than two minutes to execute. The program should be easily transportable to other IBM installations. It has, in fact, run correctly on another non-EPA IBM computer system after installation directly from tape. Non-IBM users will probably have to modify the NAMELIST inputs and perhaps other program segments where character manipulations are used.

The PRESTO-EPA-POP code is structured in a modular form to permit simple upgrading or replacement of given submodels without rewriting the entire code. Different submodels are invoked or called in changed order for scenarios other than the normal scenario. The subroutine structure of the code is shown in Figure 3.1.

There are three classes of submodels: unit response, scheduled event, and bookkeeping submodels. Unit response submodels simulate processes such as rainwater infiltration through the intact portion of the trench cap, erosion of soil overburden from the trench cover, and atmospheric transport. Such submodels are usually accessed only once during a model run and generate parameters and rates used elsewhere in the simulation.

Scheduled event submodels estimate such occurrences as the time of trench cap failure, while bookkeeping submodels include simulating water balance in the trench and radionuclide concentrations in the trench outflow and the aquifer. Output from the bookkeeping submodels is iterated annually for the simulation period. Risk evaluation bookkeeping submodels accept the cumulative or mean output from the transport portion of the code and generate doses and population risks, based on a life-table approach.

3.2 Description of Subroutine

MAIN This subroutine is the main calling program of PRESTO-EPA-POP and defines the most commonly used variables of the code, specifies dimension and common areas, and initializes variables and input control parameters. The input and output subroutines, SOURCE and OUT, are called directly by MAIN (Figure 3.1), as are the unit response model subroutines AIRTRM, and ERORF. MAIN also calculates: the vertical water velocity; retardation factors; vertical, horizontal and total transit times in groundwater (the

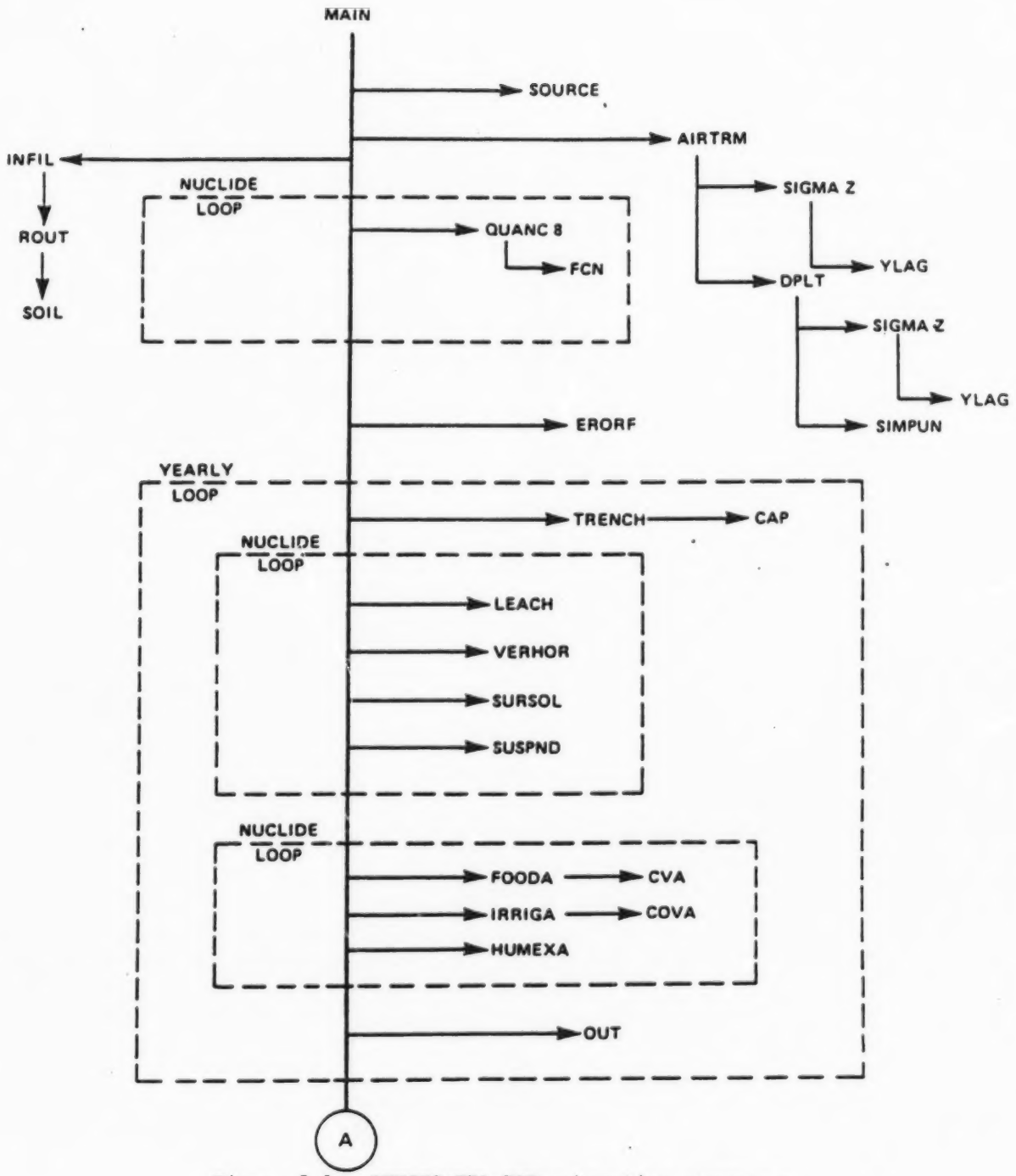


Figure 3.1. PRESTO-EPA-POP subroutine structure

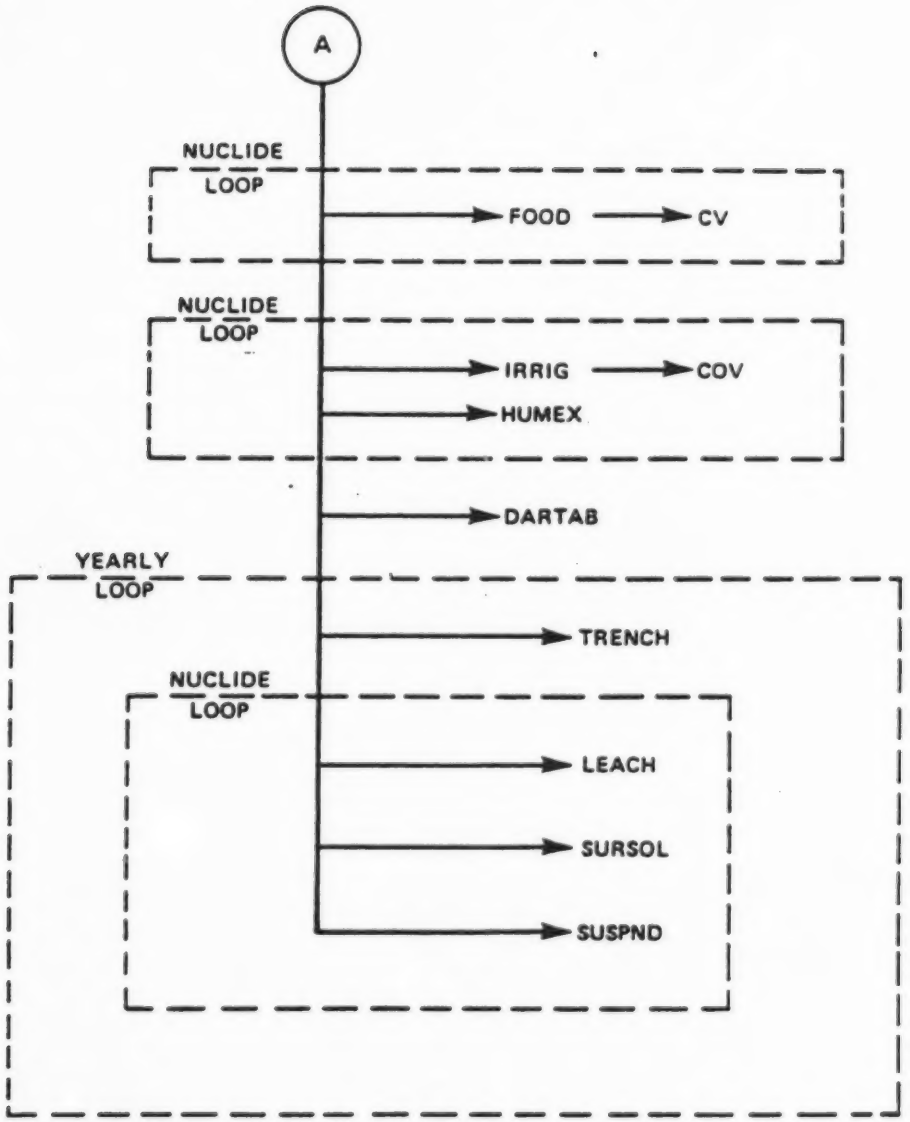


Figure 3.1. PRESTO-EPA-POP subroutine structure (continued)

transfers from trench to vertical soil column to aquifer in Figure 2.1); and the basement exposure correction factor (Section 2.2.2). The decay-dispersion correction factor, DDETA (after Hung 1981), is calculated for each radionuclide in MAIN (DDETA factor adjusts the activity output of the aquifer for the combined interactions of longitudinal dispersion and radioactive decay.) QUANC8, which is based on the eight panel Newton-Cotes rule, performs the integration to obtain the correction factor.

MAIN calls bookkeeping subroutines to calculate quantities associated with trench water balance, trench cap status, changes in land use and basement occupancy. Other subroutines called by MAIN compute amount of leaching from trench, transport of soluble surface components, atmospheric concentrations, and well concentrations. In addition, aquifer volume, hypothetical radionuclide withdrawal from well, and material balance for water in the aquifer are calculated in MAIN.

Risk evaluation submodels called from MAIN account for radionuclide concentrations in food due to atmospheric deposition and water irrigation, radionuclide intake by man. These subroutines are IRRIG, FOOD, HUMEX, CV, COV, IRRIGA, FOODA, HUMEXA, CVA, and COVA. Finally DARTAB, which creates tables of predicted health effects from radioactive effluents, is called.

The annual simulation loop and the radionuclide loop are executed a selected number of times. During a model run, MAIN may access any or all of the subroutines or functions which are listed below in alphabetical order.

Average concentration values printed in the concentration tables are computed in the MAIN Subroutine using a summation calculation within the MAXYR loop (the principal yearly iteration loop). After this loop is completed, the summed concentration values are divided by the number of years considered in the simulation and the results are printed. Maximum concentration values are identified by comparing stored concentration values to the values determined in each iteration of the same yearly simulation loop. If the new value is greater, then it, and the corresponding year number, are stored for printing in the concentration tables.

AIRTRM

This subroutine is the main calling program for the atmospheric transport submodel. AIRTRM calculates sector-averaged (22.5 degree) atmospheric exposures normalized to source strength and at wind speed, EXPOS. AIRTRM and all

its accompanying subroutines are adaptations of an interactive Gaussian plume atmospheric model, DWNWND (Fields and Miller, 1980). AIRTRM also calculates the deposition rate onto surfaces per unit source strength, DEPO. To make these calculations, AIRTRM accesses four other subroutines, SIGMAZ, DPLT, YLAG, and SIMPUN, and utilizes a number of user-input parameters including source height, H; lid height, HLID; stability class, IS; type of suitability class formulation, IT; Hosker roughness parameter, ROUGH; wind velocity, U; deposition velocity, VD; gravitational fall velocity, VG; and source to receptor distance, XG. The normalized atmospheric exposures are returned to the main program and are used in later dose and risk calculations.

CAP

This function calculates, and returns to both MAIN and TRENCH, the fraction of the trench cap that has failed. Cap failure may be either partial or total. Total failure may be caused by erosion of all overburden as calculated by ERORF. Partial failure indicates that a portion of the cap has been completely removed; the remainder of the cap is still subject to erosion. Partial failure may be caused by user input of the end points of a linear function to selectively remove all overburden from a fraction of the trench.

COV, COVA

These functions are called by subroutine IRRIG and IRRIGA to calculate radionuclide concentrations in vegetables, milk, and meat consumed by humans that may be contaminated by irrigation of agricultural crops with contaminated water. For each nuclide, COV uses the agricultural productivity of vegetation, the period of irrigation annually, the storage delay period between harvest and use for pasture grass, feed, leafy vegetables and produce, and the radionuclide decay constant.

CV, CVA

These functions are utilized by subroutines FOOD and FOODA to calculate radionuclide concentrations in pasture grass and stored feed consumed by animals, and in leafy vegetables and produce consumed by humans. CV is essentially the same as function COV, except that CV is for atmospherically deposited radionuclides and COV accounts for radionuclides deposited during spray irrigation. For each radionuclide, input data include agricultural productivity, fraction of the year vegetation is exposed to depositing radionuclides, and the delay time between harvest and consumption for stored feed, pasture grass, leafy vegetables, and produce.

DARTAB

The original DARTAB is a stand-alone program which combines radionuclide environmental exposure data with dosimetric and health effects data to create tables of predicted impacts of radioactive effluents. It had eleven subroutines and contained over 3000 FORTRAN source statements. DARTAB subroutines are RDSTOR, FACOUT, CHLOC, PREPDR, PREPRF, PREPHR, MULT, DRTAB, ORGFAC, SUMMRY, and SUMM22; these are not discussed specifically in this report. Readers interested in the original DARTAB should consult the document describing the code (Begovich et al., 1981). DARTAB has been modified slightly for PRESTO-EPA-POP so that its original main program is treated as a subroutine. Environmental exposure data are now passed in COMMON from MAIN to DARTAB's subroutines.

DARTAB makes use of dosimetric and health effects data from the methodologies of RADRISK (Dunning, Leggett, Yalcintas, 1980). RADRISK is a life-table approach to calculating the human health risk to a cohort of 10^5 people from a constant input of 1 pCi/y (0.037 Bq/y) via ingestion and inhalation for a lifetime (70.7y).

These intake conditions are approximated in PRESTO-EPA-POP by calculating an average intake over the span of the assess- ment of each type of intake. RADRISK data files are accessed directly by DARTAB.

DPLT

Subroutine DPLT, called by AIRTRM, computes a correction factor for plume depletion. To make this calculation, DPLT calls both subroutines SIGMAZ and SIMPUN.

ERORF

This subroutine uses the universal soil loss equation, USLE, developed by the U.S. Department of Agriculture (USDA 1961) to determine sediment loading for rain-driven surface erosion. Estimation methods and tabulations for factors used in USLE have been published by McElroy et al. (1976). The code user inputs all six of these factor values. The calculated erosion rate is returned to MAIN where it is converted to an annual erosion rate in meters. This erosion rate is utilized by MAIN to determine the thickness of the cap.

FCN

This function subprogram returns to QUANC8 a functional evaluation of the integral used in calculation of the aquifer decay-dispersion correction factor. The routine is written in double precision to facilitate interaction with the double precision routine QUANC8.

FOOD, FOODA — Subroutine FOOD is called only once per simulation and calculates the average concentration of each radionuclide in foods contaminated by atmospheric deposition and root uptake. The deposition input to FOOD is calculated in subroutine AIRTRM. The equations and internal parameters used by FOOD are those in AIRDOS-EPA (Moore et al., 1979). Output from FOOD is used by the subroutine HUMEX to calculate the human exposure via ingestion of these contaminated foodstuffs. Subroutine FOODA is called from MAIN each simulation year.

HUMEX, HUMEXA — Subroutine HUMEX accepts user input and receives averaged data from subroutines AIRTRM, FOOD, IRRIG, and VERHOR to calculate the average annual human exposures via ingestion and inhalation. Output from HUMEX supplies the input to the DARTAB subroutines for calculations of risk and dose and tabulation of health results. Subroutine HUMEXA is called from MAIN each simulation year.

INFIL — Subroutine INFIL, which is based on a model by Hung (1982), calculates annual infiltration through the trench cap. INFIL calls subroutine SOIL and ROUT. Inputs to INFIL include hourly precipitation, daily temperature, and various trench cap characteristics.

IRRIG, IRRIGA — Foods may be irrigated with contaminated water from either surface or groundwater sources. Input to IRRIG, which is called only once per simulation, includes the time-averaged radionuclide concentrations in well or surface water calculated by VERHOR or subroutine SURSOL, respectively. IRRIG calls function COV and uses the equations in AIRDOS-EPA (Moore et al., 1979) to calculate the time-averaged concentration of each radionuclide from direct deposition by irrigation and subsequent root uptake in foodcrops. Subroutine IRRIGA is called from MAIN each simulation year.

LEACH — Subroutine LEACH calculates the amount of each radionuclide from the homogeneous trench contents that leaves the trench each year. Losses may be via transport through the trench bottom or by overflow from the trench. There are five independent user-specified methods that may be used to calculate these amounts: the option is chosen by specifying a value from 1-5 for parameter LEAOPT. Table 2.2 lists the calculational methods corresponding to values of LEAOPT. The total-contact options, 1 and 3, assume that all of the trench contents have been in contact with water during the previous year. The immersed-fraction options, 2 and 4,

assume that the wetted fraction of the waste equals the ratio of maximum water level to the trench depth. The distribution coefficient options, 1 and 2, utilize a K_d approach to calculate the radionuclide concentrations released from the wastes to the water, while options 3 and 4 use a solubility estimate rather than K_d. If the user selects LEAOPT = 5, then a user-specified fraction of the total radionuclide concentration in the waste is lost through the trench bottom annually.

Output from LEACH is the activity leaving the trench annually for each radionuclide through the bottom of the trench and by overflowing.

OUT — This subroutine produces annual summaries for: the trench cap status; trench water balance; amount of water leaving trench; and radionuclide contents in trench water, trench overflow water, aquifer, well water, and on the ground surface. The user may choose to print these summaries for every year or less frequently by specifying the appropriate values of IPRT1, IPRT2, and IDELT in the input data deck.

QUANC8 — This subprogram is an adaptive Newton-Cotes 8-panel quadrature (Forsythe, Malcolm, and Moler, 1977). The integral to be evaluated is specified by the function FCN.

ROUT — Subroutine called by INFIL.

SIGMAZ — This subroutine is called by both AIRTRM and DPLT to compute the vertical dispersion parameter, SIGZ. Depending on the choice of value given to parameter IT in the input data set, SIGMAZ will calculate SIGZ by one of eight schemes, shown in Table 3.1. Necessary input data include the downwind distance, XG, stability class, IS, Hosker roughness parameter, ROUGH, and lid height, HLID. Other data necessary for Lagrangian interpolations (by function YLAG) are contained internally in SIGMAZ and need not be input by the user.

SIMPUN — This subroutine, originally written by Barish (1970), uses Simpson's rule to integrate along the ground level centerline of the atmospheric plume to compute the depletion fraction. All input to SIMPUN is supplied by DPLT, the subroutine that calls SIMPUN and to which the results are returned.

SOIL — Subroutine called by ROUT.

SOURCE

Subroutine SOURCE performs most of the necessary inputs of information to initialize and quantify transport parameters, except those required for Subroutine INFIL. Data concerning program control, climatic description, trench description, aquifer description, atmospheric description, site-surface description, and radionuclide description are read in by SOURCE from unit 5, stored on unit 26, and reread. SOURCE also prints out these data before any calculated results are output.

SURSOL

Subroutine SURSOL computes the amount of soluble radionuclide that enters the stream annually. Input variables to SURSOL include the average depth of active exchange in the soil, ADEPTH; the average downslope distance to the stream, PD; the cross slope extent of the spillage, EXTENT; the average annual infiltration, SINFL; the bulk density of soil, BDENS; the amount of spillage, SOAM; and the surface soil distribution coefficient, XKD. Variables output from SURSOL include SSTREM, SDEEP, and CW, the amounts of radionuclide going to the stream and the deep soil layers; and the radionuclide concentration in the interstitial water of the contaminated surface region, respectively.

SUSPND

This subroutine calculates the above trench atmospheric source term from the ground surface by two methods, a time-dependent resuspension factor and a resuspension rate due to mechanical disturbances. Input variables include the current year of simulation and radionuclide, the spatial area of the contaminated surface, SAREA; the radionuclide concentration on the ground surface, GNDCON; the beginning and ending years of mechanical disturbances, IRRES1 and IRRES2; the resuspension rate, RR; and the wind velocity, U. SUSPND assumes that all radionuclides to be resuspended were deposited on the soil surface at simulation time zero. Material may be added to the atmospheric source term through two methods: resuspension by wind from surface soil, YSO1, and resuspension by mechanical disturbance, YSO2. The resuspension factor calculated uses the empirical equation of Anspaugh et al. (1975).

The atmospheric source term, YSO (referred to previously as algebraic variable Q), is returned to MAIN and is used along with χ/Q to calculate the air concentration of each radionuclide available for deposition onto foodstuffs and for inhalation by the general population. The value of χ/Q is calculated by AIRTRM.

TRENCH

Subroutine TRENCH determines the trench water balance. Input variables include trench dimensions, porosity and permeability of trench contents, trench water volume from the previous year, length of the saturated zone, annual precipitation and infiltration, and the current year of the simulation. Output from TRENCH includes the maximum depth of water in the trench, the volume of water in the trench, volume of water overflowing the trench, and water volume lost from the bottom of the trench.

The overflowing amount of water, VOLO, is calculated by comparing the maximum water depth to the trench depth and overflowing any amount greater than trench volume. The variables VOLO, VOLB, OLDWAT, and DMAX that quantify overflow, bottom loss, water level during previous year, and maximum water depth in trench, respectively, are used by the subroutine LEACH, discussed previously.

VERHOR

This subroutine calculates and decays the amount of each radionuclide, AQAM, that reaches the irrigation/drinking water well in a given year. Variables evaluated elsewhere in the code and input to VERHOR include the current year of the simulation, NYEAR; transit time from the trench to the well, ITIME; the volume of water leaving the trench bottom, VOLB; the amount of each radionuclide leaving the bottom of the trench, POLB; the amount of radionuclide reaching the aquifer from the contaminated surface region, SDEEP; and the radioactive decay constant, DECAY. This amount is corrected in VERHOR by the decay-dispersion correction factor, DDETA, adapted from Hung (1981).

YLAG

This function performs a Lagrangian interpolation of the SIGZ block data and is called by subroutine SIGMAZ. The original program was written by Brooks and Long (1970) and adapted for use here. All input data are supplied by SIGMAZ.

XPRESS

Computes exponential decay factors to be used repetitively in the nuclide loops. This subroutine saves a substantial amount of computing time.

APPENDIX D

Peer Review Panel Comments

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

JUL 13 1984

Mr.
Environmental Protection Agency
401 M Street, SW
Washington, D.C. 20460

Dear Mr. :

I am glad to inform you that the enhancements and modifications to the PRESTO-EPA model resulting from the valuable input provided by the Peer Review, in which you participated, have been completed. Detailed documentation of the new capabilities of PRESTO is being prepared at the present time, as well as the Peer Review Report. In this letter, I just want to highlight the work we have done.

1. Extension for Modeling Arid Scenarios (Partially Saturated Flow):

PRESTO now has the capability of modeling the migration of nuclides from the trench to the aquifer under partially saturated conditions. In this extension, the vertical water velocity and the vertical retardation factor are calculated as a function of the saturation of the soil. In particular, if the saturation of the soil has the value of one, the equations correspond to the saturated flow scenario. The saturation of the soil can be calculated within PRESTO using the relationship between the water velocity and the hydraulic conductivity. However, this calculation will be overridden if a more precise estimate is available and specified in the input data.

2. Leaching Option for Partially Saturated Conditions:

Leaching Option 2 has been modified. Using the trench infiltration rate and the trench permeability a contact time factor is calculated, such that its value is never greater than 1. The contact time factor is then used to derate the leached trench water concentration.

3. Correction of Conservatism in Basin Residual Modeling:

The same methodology, already used in PRESTO to calculate transit times in the aquifer from the trench to the local use point, is now used in the

Basin Residual Submodel to calculate transit times from the local use point to the basin stream. The distance from the well point to the stream is a new item in the input data. This part of the code also (1) accounts for decrements of the flow to the stream due to withdrawals of well water for community use and (2) permits the user to allow some percentage of the ground-water flow to bypass or underflow the basin stream.

4. Farming over the Trench Scenario:

A new option has been developed to simulate farming over the trench after loss of institutional control of the disposal area. If this option is chosen, the model will calculate the bio-intrusion directly through the trench cover and into the waste and the subsequent uptake of radionuclides by the roots of the vegetation. The soil-to-plant transfer factor is utilized for the portion of root systems that are directly extended into the waste. The contaminated vegetation are added to that vegetation contaminated from other PRESTO pathways for human consumption. A provision is also included to calculate the effect from the biological decay of the contaminated vegetation which are converted into contaminated topsoil. This option is activated by the user.

5. Container/Solidification Delay:

Leaching no longer must start the first year of simulation. Holdup and delay due to containment by packaging may be simulated by the introduction of a holdup factor that is applied to the trench water concentration. The holdup factor stays at level zero until the estimated date the container starts to fail. Then, it climbs linearly to a value of 1 during the estimated container failure time, and stays equal to 1 after the container has failed completely.

6. Radionuclides Concentration in Vegetation:

The issue of radionuclide concentration calculations in vegetation raised at the Peer Review Meeting was further studied and discussed within EPA, with EPA contractors and with participants of the Peer Review. The following conclusions were reached and the changes to the code were developed when necessary.

PRESTO currently calculates both the tritium concentration due to atmospheric deposition and the tritium concentration due to the use of contaminated irrigation water. This methodology was found comparable to other methodologies and no changes were made.

Because most carbon uptake by plants is from atmospheric carbon dioxide and very little is from irrigation, we have deleted C-14 transfer to plants via the water pathway.

The general formula used to calculate the radionuclide concentration in vegetation (except tritium and carbon C-14) has been revised as suggested in the Peer Review, and now it includes a translocation factor similar to the one used in the work of Baker, Hoenes and Soldat (1976).

7. Radionuclide Decay During Facility Operation:

Decay correction factors are now calculated in PRESTO to account for the decay of the radionuclide inventory during the operational period of the facility.

8. DARTAB Output:

Unneccessary output from subroutine DARTAB has been blocked.

9. Area Source Term for the Ground Water Transport:

In the Maximum Individual Dose version of PRESTO, the point source term for the ground water transport has been changed to an area source term to reflect the fact that percolation occurs over the entire extent of the trench bottom.

10. Area Source Term for the Air Path-Way:

The point source term for the air path-way has been changed to an area Source Term.

We are more than three months behind the schedule we originally set to complete the Peer Review because of contract admimistration matters. These difficulties have been cleared up and work on the Peer Review Report, documentation and user's manual should procede in an orderly manner henceforward. We should complete the Peer Review Report in the next two months followed by the documentation and user's manual several months later.

During the interim, we have learned a lot about PRESTO through daily use (several hundred test and production runs with PRESTO or its progeny). Phil Cuny has, for our own (ORP) internal use, prepared a souped up, faster-running version of PRESTO with slimmed down (only 10 nuclides) standardized data sets for the Southeast, Northeast and Southwest scenarios for testing and sensitivity runs.

Also, we found that a quality assurance audit helps tremendously to clean up and better understand a model. We also found that it is no guarantee that all bugs have been exterminated. Twice during one montn after we had "completed" our final production runs, we found through sensitivity testing very subtle but very important logic errors embedded within the original code. As a result, we made three sets of "final" production runs. Therefore, I would strongly recommend against using any versions of PRESTO which have not been obtained from Phil Cuny, our ADP Manager.

We are currently vigorously testing and analyzing the sensitivity of PRESTO. This program includes evaluating: (1) sensitivity of a given parameter; (2) sensitivity to a general change in conditions; (3) sensitivity to parameter values which are particularly uncertain; (4) basic tests of the PRESTO model and submodels; and (5) special tests. We will make our report on this evaluation available to you upon its completion.

As we mentioned at the meeting, the U.S. Geological Survey (USGS) has agreed through an Interagency Agreement to evaluate output from the ground-water transport section of PRESTO. They may use output from their own ground-water modeling efforts and other means or methods they may choose to make this evaluation. They will evaluate the output from PRESTO for Southeast (humid, permeable), Northeast (humid, low permeable), and Southwest (arid, permeable) climatic and hydrogeologic scenarios., We have stressed to the USGS that our modeling is intended to be generic and under average or typical conditions but that we have attempted to use realistic data. This USGS will mainly be evaluating ground-water transport from point of infiltration at the trench to point(s) of release to a receptor. We have also invited them to evaluate any other section they may wish to. Their evaluation report will be made available to you upon its completion and release by the USGS.

Some participants in the review missed the point that PRESTO is intended for use in comparing different disposal method/waste stream combinations on a generic basis under three different hydrogeologic scenarios. This was probably due to the fact that we used the names Barnwell, West Valley and Beatty, to designate Southeast, Northeast and Southwest scenarios. We have

since expunged all references to specific sites by name in PRESTO input and output and will be doing so in the final documentation and user's manual.

Much was said about the uncertainity of data for certain input parameters. We cannot really cure this problem as part of our developing PRESTO. We have, however, taken steps to check the data values which we will be using with those used by others knowledgeable on the particular subject. Our staff or our contractor staff have contacted the geotechnical and modeling staffs of the Nuclear Regulatory Commission (NRC), Savannah River Laboratory (SRL), Chem-Nuclear, Inc., U.S. Ecology Inc., USGS, and Battelle Northwest to compare and, in some cases, revise input values we are using for radionuclide K_ds and uptake rates and hydrogeologic input parameters. In most cases, the values we are using are, I believe, comparable to those used by others doing transport modeling on a generic basis. There was some disagreement on aquifer input which should be used for the Southeastern and Southwestern scenarios. We are using the values furnished to us by the USGS for our production runs. We are also making sensitivity runs to test the effects of other values which were suggested and will make the results of the comparisons available in our report on sensitivity tests.

I look forward to hearing from you and thank you again for your candid thoughts about PRESTO-EPA.

Sincerely Yours,

G. Lewis Meyer
Project Leader
Low-Level Waste Standards Project
Criteria and Standards Division (ANR-460c)
Office of Radiation Programs

GLM/ct

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

GENERIC COPY OF LETTER SENT TO ALL ATTENDEES OF EXPERT REVIEW HELD ON FEBRUARY 7 & 8, 1984, AT AIRLIE HOUSE, AIRLIE, VIRGINIA

February 27, 1984

ATTENDEE'S NAME
ATTENDEE'S ADDRESS

Dear :

We would like to thank you for assisting the Environmental Protection Agency (EPA) in the review of PRESTO-EPA, our model for estimating the potential impact from the land disposal of low-level radioactive wastes (LLW). Your comments at the Expert Review were extremely helpful to us by pointing to areas which were unclear and needed improvement. We are working on making the changes to the various parts of PRESTO-EPA which were put forth during the Expert Review. Attached is Enclosure 1 which enumerates those changes.

You will recall that during the Expert Review, some people expressed a desire to submit to us their written comments about PRESTO-EPA after the Expert Review had been completed. If you plan to do this, please send your written comments within the week so that we can include them in the report on the Expert Review of PRESTO-EPA.

Should you wish a copy of the verbatim, original transcription of the taping of the Expert Review as delivered to EPA by the court reporter, write or call for:

Docket # R-82-1
Central Docket Section [LE-130]
U.S. Environmental Protection Agency
401 M Street, SW
Washington, DC 20460
(202)382-7548 FTS-382-7548

Vern Rogers, President of Rogers & Associates Engineering Corporation, has asked that we send to you the attached ERRATA for the PRESTO-DEEP document which Vern distributed at the Expert Review meeting in February.

We look forward to hearing from you and thank you again for your candid thoughts about PRESTO-EPA.

Sincerely,

G. Lewis Meyer
Project Leader
Low Level Waste Standard

ENCLOSURE 1

of

Listing Model/Submodel Revisions & Improvements
and Data Collection and Revision, Based on Recommendations of
PRESTO Peer Review, February 7-8, 1984

MODEL/SUBMODEL REVISIONS AND IMPROVEMENTS

1. Improve Capability (RAECo) for Modeling Arid Scenarios:
Improvements are needed in modeling the percolation of waters infiltrating into the trenches from the trench bottom to the aquifer through unsaturated or partially saturated geologic media often found in arid climates. RAECo should prepare and test an integrated or stand alone submodel which will properly simulate the vertical transport of water and radionuclides under these conditions and upgrade the documentation to reflect this modificatin. Careful consideration should be given to preparation of input parameters and data requirements.

2. Improve Waste Leaching Option Under Partially Saturated Conditions (RAECo): Improvements are needed in how LEOPT (Option 2) handles the leaching of wastes in the trenches under partially saturated conditions. Please improve Option 2, LEOPT so that it handles partially saturated leaching more realistically.

3. Correcting Conservatism in Basin Residual Modeling (Inter Systems):
The basin residual model presently allows the release of unconsumed radionuclides passing a ground water use point (i.e. well) directly to a stream without the delay from addition transport through an aquifer or retardation from geochemical exchange with the aquifer. Add a distance factor from the well to the stream and recompute the transport of "residual" radionuclides passing the well to the stream using the horizontal component of VERHOR including the Hung dispersion correction factor.

4. Add Farming Impact Submodel (RAECo): Savannah River Laboratories, in their analyses of the potential impacts of their shallow land disposal operations for LLW, have determined that farming over the trench after loss of institutional control of the disposal area could have the greatest health impact of any exposure pathway to the public. PRESTO-EPA presently does not handle this farming scenario very well. Upgrade the farming impact submodel to include as many of the features which the SRL DOSTOMAN model currently includes. This upgrading should include, if possible, use of differential root depths in radionuclide uptake from the trenches. We have already furnished to the contractor (RAECo) a report which describes the SRL approach to modeling farming impact. Because of the technical complexity of this submodel, consideration of having it function outside of the overall PRESTO-MID models may be considered. SRL has agreed informally to cooperate with us on development of this module. I will work out details on protocols for contacts with SRL staff and inform ORP and contractor staffs. No contact should be made with SRL until I have forwarded this information.

5. Add Container/Solidification Delay and Release of Activity Turn-On Time Factors for Wastes (RAECo): Currently, PRESTO makes radionuclides in wastes available for leaching immediately after the site is officially closed. The reviewers correctly pointed out that this is probably incorrect and that some holdup and delay due to containment by packaging occurs. Add the capability to the leaching subroutine of PRESTO to allow the radionuclides in the waste to remain in place until a release time is specifically stated. In addition, this factor should include a mechanism for a progressive failure rate for the containers/packages. Utilization of this "container delay" and "turn-on time for relese of activity" will require preparation of typical "release times" for each waste form.

6. Reevaluate H-3 and C-14 Uptake Rates in Foodchain Transfer Coefficients (contractor undetermined at this time): Several reviewers said that PRESTO's current H-3 and C-14 foodchain transfer coefficients overestimate foodchain uptake by 5 times to two orders of magnitude (depending on the nuclide). This potential overestimate should be evaluated and corrected if necessary. Chris Nelson is checking on this problem and will determine whether contractor support is necessary.

7. Add Correction Factor for Radionuclide Decay in Wastes During Facility's Operational Period (RAECo): Currently, PRESTO begins decay of radionuclides in waste at close of a facility's operational period. This may lead to an overestimate of potential radiological impact, especially for short-lived radionuclides (i.e., half-lifes less than 13 years). Add a correction factor for radionuclide decay during the facility's operational period. This factor should be placed in the accounting model, if possible.

*8. Do Not Print Selected Output from PRESTO (Inter Systems): Population doses for "selected individual" and "mean individual" currently are printed by PRESTO output but are not used in any present or planned output. Delete these two data output sets from printed PRESTO-EPA output.

DATA COLLECTION AND REVISION

1. K_ds for All Radionuclides (Envirodyne, RAECo and USGS): Although we are currently modeling three different hydrogeologic and climatic scenarios, there is a very close similarity between K_ds for most radionuclides for all three scenarios. A final reevaluation of K_ds should be made for each radionuclide on a site-by-site scenario basis. This will require participation and cooperation between Envirodyne, RAECo and USGS. Envirodyne will take lead in contacting sources for K_ds. K_ds will be submitted to Jim Neiheisel and Cheng Hung for review.

2. Hydrogeologic and Climatic Scenario Data (Envirodyne): The "correctness" or "appropriateness" of certain hydrogeologic and climatic data have been questioned. Operators of commercial sites have stated that some of our site hydrogeologic data are "too conservative." We have found from operating PRESTO that travel times under unsaturated arid conditions are greatly overestimated. We should, therefore, carefully reevaluate all existing hydrogeologic and climatic data prior to making new production and accounting model runs. Point 1:

the data or confirmatory information needed for this reevaluation must be obtained from a variety of sources. Point 2: output from PRESTO is often very sensitive to the input data. Therefore, I am requesting that Envirodyne take the lead on this subtask by furnishing a qualified hydrogeologist to reevaluate and, as necessary, collect new data. He will be responsible for contacting the USGS (all three sites and scenarios), U.S. Ecology (arid or Beatty site), Chem Nuclear (humid permeable scenario or Barnwell site), and Savannah River Lab (humid permeable scenario). I will establish initial contacts with these organizations prior to Envirodyne conducting these site-by-site data evaluations.

3. Farming Scenario Data (RAECo and Envirodyne): A farming impact submodel will be developed as described in the previous section on Model Development and Improvement. Data for this model must be acquired. A likely source for this information is the Savannah River Laboratory. RAECo will take the lead in collecting this data with support, as necessary, from Envirodyne. Initial contact with SRL will be made by EPA prior to RAECo contacting them.

4. K_ds for Waste Streams (Types) (RAECo): Questions were raised about how realistic the waste K_ds (partioning coefficient, as per one reviewer) used in PRESTO were. The waste K_ds currently being used in PRESTO should be reevaluated in light of new data that is available.

5. New Population for Humid Sites/Scenarios (EPA): Based on comments of reviewers and our own internal decisions, we are going to revise the populations currently being used at the humid low permeable scenario (West Valley site) and humid permeable scenario (Barnwell site) to make our analyses more generic. These new data will be developed by EPA staff with consultation of all parties.

6. Renaming of Scenarios: Based on the unanimous opinion of all reviewers and the EPA support team, the use of site specific names with examples of input and output for the different hydrogeologic and climatic scenarios (i.e., Beatty for arid scenario) is confusing and distracts reviewers and potential users away from PRESTO-EPA's intended use as a generic model. Therefore, all contractors - man your word processors and go on a "search and change" mission for Barnwell, Beatty and West Valley - in the PRESTO documentation, input, output, data sets, and various reports! Use caution and common sense when you get to the reports or sections describing the sources of the data. If there are any questions on this, please contact me.

APPENDIX E

Considerations for IBM-PC/AT Versions

Considerations for an IBM-PC/AT Version of PRESTO

Although the target hardware identified for this study was the AECB's HP1000, some interest into the possibility of using the model in an IBM-PC/AT environment became apparent during the course of this study. This discussion is meant to identify considerations under this scenario based on our existing familiarity with PRESTO. The areas of concern for software in any hardware environment are typically:

- Memory
- Turnaround (execution speed)
- Input requirements
- Output requirements.

PRESTO requires approximately 1.4 Mbytes of memory in its currently configured condition while most IBM-PC/AT running under PC-DOS typically have only 600 kbytes available. In order to get PRESTO to "fit" a number of options (or combinations of the options) are available.

1. Reduce array storage - PRESTO is dimensioned to handle up to 40 nuclides for 10,000 years. By reducing this to 10 nuclides for 1000 years an IBM-PC/AT could accomodate the model. Other combinations are possible (e.g., perhaps 1 nuclide for 10,000 years), however, it must be recognized that a major drawback to such an approach is its inflexibility to handle a variety problems (e.g., problems that may exceed either of the fixed dimensions).

2. Reduce the size of the program itself. PRESTO performs many calculations which are not of primary interest to AECB. By eliminating these sections of the program and their associated storage a larger dimensioned PRESTO version could be installed.

3. Change selected array storage from central memory to disk storage. This option may impact the turnaround as discussed below.

To evaluate turnaround on the HP1000, a reduced size problem was run on an IBM-PC/AT by reducing array sizes. Turnaround for 10 nuclides for 1,000 years was found to be of the order of 10 minutes. Although the relationship between execution speed and simulation time period or radionuclide inventory is not exactly linear (due to initialization, I/O, etc.), it is safe to say that, for most deterministic problems, turnaround would be adequate, on the order of hours. Option #3 identified may increase turnaround due to additional I/O, however, it is unlikely that this would be significant.

Input for an IBM-PC/AT would require either an input pre-processor (similar to that proposed under Scenario 2) or familiarity with a text editor and data formats.

The output capabilities of the IBM-PC/AT environment should be examined for their suitability in handling typical PRESTO outputs. Typical dot matrix printer speeds for such environments are quite slow and may dictate the need for a faster (probably laser) printer. The size of potential outputs will also dictate the suitability of using editors to preview results.

An additional consideration is the fact that the choice of IBM-PC/AT hardware would preclude the possibility of developing a probabilistic capability.

The tasks identified under the scenarios described in the report would, for the most part, not change significantly for IBM-PC/AT target hardware. The addition of mechanisms/pathways, construction of input and out pre-processors would remain virtually identical. Only the installation task identified under Scenario 1 would change

significantly. Segmentation of the code on the HP1000 would not be required although an evaluation of approaches to resolve memory deficiencies and the implementation of the optimum approach would take its place. The QA and instruction portions of the task would also remain virtually the same. It is therefore unlikely that the level of effort associated with the IBM-PC/AT scenario would be significantly different from that of the HP1000.